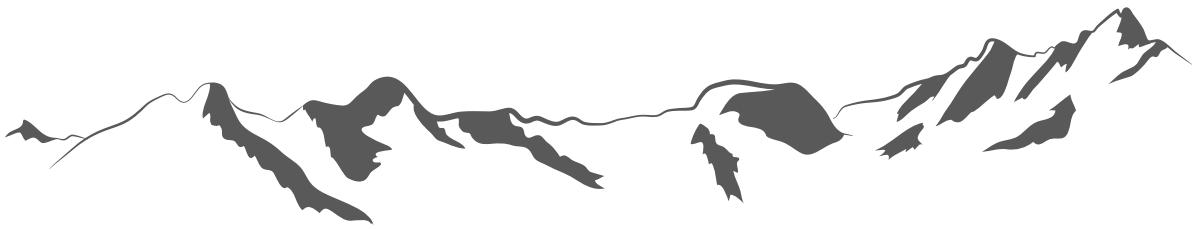
iWOE25

25th International Workshop on Oxide Electronics

1st – 3rd October 2018

Les Diablerets, Switzerland



Workshop Program

Full booklet of abstracts available at www.iwoe25.org

25th International Workshop on Oxide Electronics

1st – 3rd October 2018

Les Diablerets, Switzerland

International committee

Charles H. Ahn, Yale University
Ariando, National University of Singapore
Chang-Beom Eom, University of Wisconsin-Madison
Masashi Kawasaki, University of Tokyo
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Sponsors

Asylum Research, an Oxford Instruments company
AIP APL Materials
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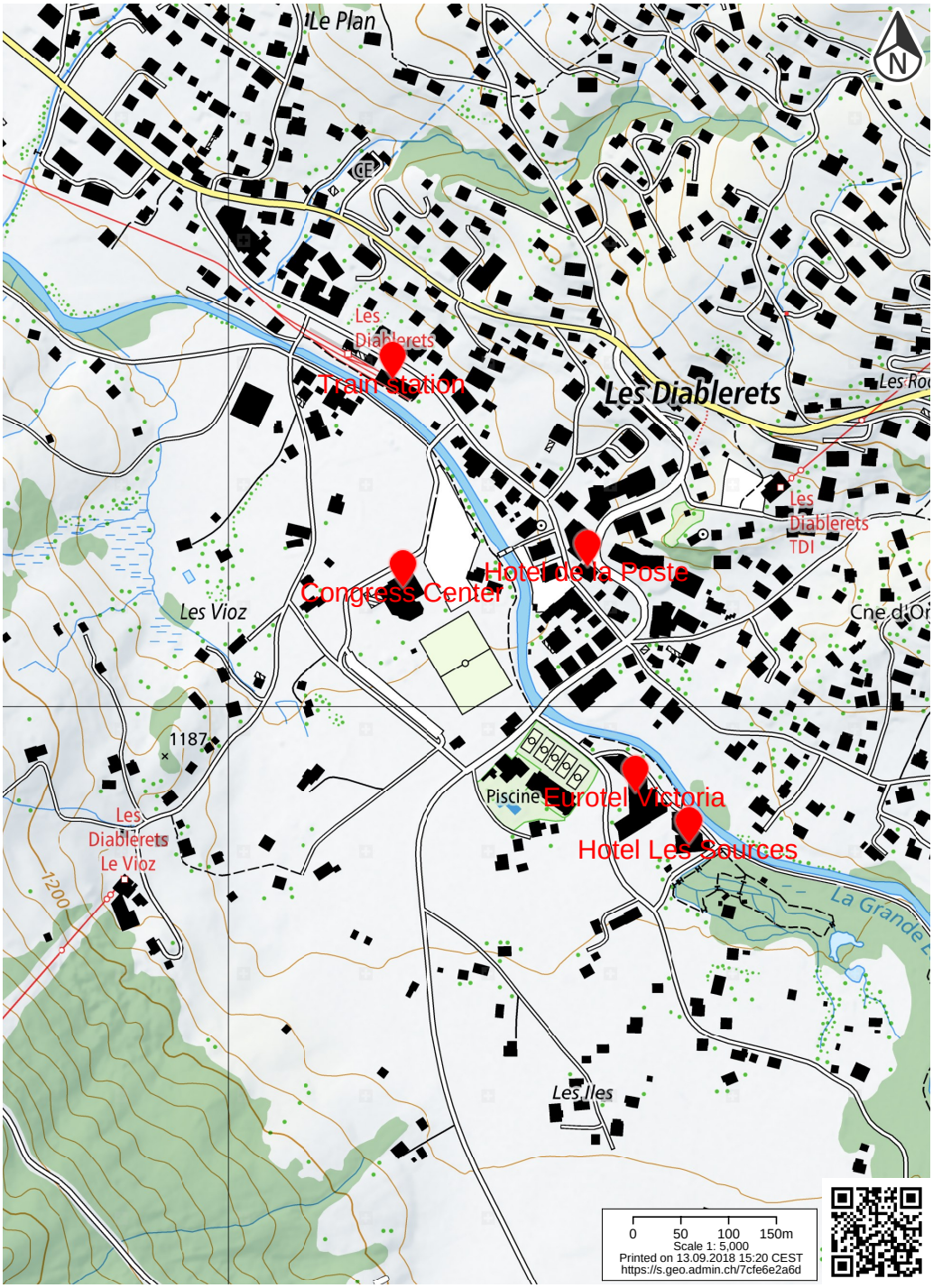
VENUE

The workshop will be held at the Congress-Center at Les Diablerets, Switzerland.
The participants will be lodged at the EUROTEL-Victoria and Hôtel Les Sources.
Both hotels and the Congress-Center are about 10 minutes walk from the train station "Les Diablerets".



WORKSHOP PROGRAM

Sunday, September 30, 2018

17h00 Registration
19h30 Dinner

Monday, October 1, 2018

08h00 Registration
08h45 Welcome and Opening Remarks

Detection of Symmetry Breaking

chair: Philippe Ghosez (*Université de Liège)*

9h00 **Patrick Maletinsky** (*University of Basel*)
Single spin magnetic sensing of mesoscopic condensed matter systems
9h30 Tobia Nova (*MPI Hamburg*)
Light-induced symmetry breaking in $SrTiO_3$
9h45 Gustau Catalan (*ICREA -ICN2*)
Breaking not-so-bad: fracture flexoelectricity
10h00 **Woo Seok Choi** (*Sungkyunkwan University*)
Ferroelectricity in 1D tetrahedral chain network via combined polar distortion

10h30 coffee break

Collective States in Transition Metal Oxides

chair: Charles Ahn (*Yale University)*

11h00 **Nicola Spaldin** (*ETH Zürich*)
Connecting ferroelectricity and superconductivity in $SrTiO_3$
11h30 Nicolas Bergeal (*Université Pierre and Marie Curie*)
Superfluid stiffness in oxide interfaces
11h45 Diogo Vaz (*CNRS, Thales*)
Enhanced spin-to-charge conversion through topological states in $SrTiO_3$-based two-dimensional electron gases
12h00 **Rui Peng** (*Fudan University*)
Revealing the role of the interface in the high-temperature superconductivity of single-layer FeSe/$SrTiO_3$

12h30 lunch break

Poster Session A

chair: Jean-Marc Triscone (*Université de Genève)*

14h00 poster session

Ruthenates

chair: Ralph Claessen (*Universität Würzburg)*

15h30 **Antoine Georges** (*The Flatiron Institute - Collège de France*)
Sr_2RuO_4: a precision laboratory for electronic correlations

16h00 Sara Ricco (*University of Geneva*)
In-situ strain-tuning of the metal-insulator-transition of Ca_2RuO_4 in angle-resolved photoemission experiments

16h15 Andrew Millis (*The Flatiron Institute - Columbia University*)
Electron-lattice coupling in correlated electron materials: Ca_2RuO_4 and beyond

16h30 25^{th} anniversary of the iWOE

18h00 **Hideomi Koinuma** (*University of Tokyo*)
Smart Combinatorial Drone for exploring a new frontier of oxide and molecular electronics

18h15 iWOE prize award ceremony

18h30 aperitif

20h00 dinner

Tuesday, October 2, 2018

Complex Oxide Interfaces

chair: Darrell Schlom (*Cornell University)*

8h45 **Karin Rabe** (*Rutgers University*)
Charge transfer and charge order in functional perovskite superlattices from first principles

9h15 Gabriele De Luca (*University of Zürich -ETH Zürich*)
Real-time observation of polarization emergence in ultrathin ferroelectric oxide heterostructures

9h30 Nagarajan Valanoor (*University of New South Wales*)
Topological transitions in ultrathin ferroelectric films

9h45 Nicolas Gauquelin (*EMAT - Antwerp*)
Electron microscopy study of the Metal-Insulator Transition in nickelate superlattices

10h00 **Naoya Shibata** (*University of Tokyo*)
Direct electromagnetic field imaging of interfaces by advanced STEM

10h30 coffee break

Spin-Orbit Coupling at Polar Surfaces and Interfaces

chair: Manuel Bibes (*CNRS - Thales)*

11h00 **Phil King** (*University of St Andrews*)
Maximal Rashba-like spin splittings and intrinsic Stoner instabilities at polar surfaces of delafossite oxides

11h30 Alexander Demkov (*University of Texas*)
A theoretical investigation of graphene on a polar $SrTiO_3$ (111) surface

11h45 Marco Salluzzo (*CNR-SPIN*)
Orbital reconstruction and spin polarization in (100) and (111) $LaAlO_3/SrTiO_3$ and $LaAlO_3/EuTiO_3/SrTiO_3$ q2DEG

12h00 **Karsten Held** (*TU Wien)*
Ferromagnetism and quantum anomalous Hall state in $SrRuO_3$ (111)

12h30 lunch break

Oxides and Their Functionalities

chair: Guus Rijnders (*University of Twente*)

14h00 **Nazanin Bassiri-Gharb** (*Georgia Institute of Technology*)
Antiferroelectric $PbZrO_3$ thin films with multiple phase transitions

14h30 Taro Hitosugi (*Tokyo Institute of Technology*)
A high Li-ion conductivity at solid-electrolyte and electrode interfaces: introducing oxide epitaxial thin-film technology to battery research

14h45 Jon-Paul Maria (*Pennsylvania State University*)
All-oxide IR devices based on high-mobility CdO thin films

15h00 **Amalia Ballarino** (*CERN*)
Superconducting materials for accelerators: an overview of state-of the art performance and future needs

15h30 coffee break and group photo

Metal-Insulator Transitions and Mott Physics

chair: Chang-Beom Eom (*University of Wisconsin-Madison*)

16h00 **Xiaoxing Xi** (*Temple University*)
Nature of the metal-insulator transition in few-unit-cell-thick $LaNiO_3$ films

16h30 Philipp Scheiderer (*Universität Würzburg*)
Tailoring materials for Mottronics: excess oxygen doping of a prototypical Mott insulator

16h45 Sophie Beck (*ETH Zürich*)
Metal-Insulator Transition in thin films and multilayers of early transition metal oxides from DFT+DMFT

Poster Session B

chair: Stefano Gariglio (*Université de Genève*)

17h00 poster session

20h00 conference dinner

Wednesday, October 3, 2018

Complex Oxide Materials Design

chair: Chris Leighton (*University of Minnesota*)

8h45 **James Rondinelli** (*Northwestern University*)
Valence precision and transparent band conductors in complex oxides

9h15 Jaap Geessinck (*University of Twente*)
Charge transfer at the $LaCoO_3$-$LaTiO_3$ interface

9h30 Hari Nair (*Cornell University*)
Growth of superconducting Sr_2RuO_4 thin films

9h45 Gervasi Herranz (*ICMAB-CSIC*)
In-situ imaging of electric field-induced ferroelastic domain motion in $SrTiO_3$

10h00 **Yoshinori Tokura** (*RIKEN - University of Tokyo*)
Emergent properties of Dirac and Weyl semimetals of iridates

10h30 coffee break

Topological Textures in Oxides

chair: Marc Gabay (*Université Paris-Sud)*

11h00 **Andrea Caviglia** (*Delft University of Technology*)
Berry phase engineering at oxide interfaces

11h30 Kei Takahashi (*RIKEN*)
Quantum transport in the films of a magnetic semiconductor $EuTiO_3$

11h45 Lingfei Wang (*Seoul National University*)
Ferroelectrically tunable magnetic skyrmions in ultrathin oxide heterostructures

12h00 **Xiaoqing Pan** (*University of California*)
Effects of ferroelectric polarization at oxide interfaces

12h30 poster award ceremony
12h40 closing remarks
12h45 lunch

Presentations:

Invited Speakers	25 mins + 5 mins Q&A
Oral Contributions	12 mins + 3 mins Q&A
Posters	Poster boards (116 cm x 116 cm) can accomodate an A0 print in portrait or lanscape orientation.

Poster Session A

A1	Bharathi Rajeswaran (*Indian Institute of Science, India*) Unraveling the Enhanced Transition Characteristics of Thermochromic VO_2 Thin Films for Energy Efficient Smart Windows
A2	Chadol Oh (*Pohang University of Science and Technology, Republic of Korea*) All inorganic electrochemical transistor with correlated oxides for low power and thermally stable artificial synapses
A3	Iwao Kawayama (*Osaka University, Japan*) Characteristics of Laser-Induced Terahertz Emissions from Gallium Oxide Surfaces
A4	Jongyoon Park (*University of Tokyo, Japan*) Selective gas sensing using WO_3 nanoparticles and zeolites hybrid structure for human cutaneous gas sensors
A5	Nicola Manca (*Università degli studi di Genova, Italy*) Micro-mechanical resonators powered by oxides' solid state phase transitions: a VO_2-based micro-engine
A6	Yonggang Zhao (*Tsinghua University, China*) Magnetoresistance behaviors of conducting filaments in resistive-switching NiO with different resistance states
A7	A. P. Nono Tchiomo (*MPI Stuttgart, Germany*) Growth and characterization of epitaxial La-doped $BaSnO_3$ thin films grown by pulsed laser deposition
A8	Alexander A. Demkov (*University of Texas, USA*) Monolithic integration of patterned $BaTiO_3$ thin films on Ge wafers
A9	Andreas Klein (*Technische Universität Darmstadt, Germany*) The Fermi energy in oxides: Assessing and understanding the limits using XPS
A10	Céline Lichtensteiger (*University of Geneva, Switzerland*) *InteractiveXRDFit*: a new tool to simulate and fit X-ray diffractograms of oxide thin films and heterostructures
A11	Daniel Putzky (*MPI Stuttgart, Germany*) Epitaxial growth of high quality $DyBa_2Cu_3O_{7-\delta}$ using Atomic Layer by Layer Molecular Beam Epitaxy
A12	F. Gunkel (*RWTH Aachen University, Germany*) Epitaxially stabilized phase and oxygen vacancy-ordering in cobaltite (double-)perovskite thin films
A13	R. de Andrés Prada (*University of Fribourg, Switzerland*) Deposition and Nanofabrication of All Perovskite $YBa_2Cu_3O_{7-y}$/Ferromagnetic/ $YBa_2Cu_3O_{7-y}$ Josephson Junctions
A14	Hugo Meley (*University of Geneva, Switzerland*) $LaVO_3$ Thin Films under Epitaxial Strain
A15	Jegon Lee (*Sungkyunkwan University, Republic of Korea*) Stoichiometry and epitaxial strain control of electrocatalytic activity in Ruthenate thin films
A16	Jos E. Boschker (*Leibniz-Institut für Kristallzüchtung, Germany*) Effect of symmetry mismatch on the heteroepitaxial growth of T-Nb_2O_5 on $SrTiO_3$
A17	M. E. Bernal (*ICMAB-CSIC, Spain*) Epitaxial growth of La_2NiMnO_6 thin films on $SrTiO_3$ by RF Sputtering
A18	M. Zapf (*Universität Würzburg, Germany*) Domain matching epitaxy and modified interfacial layer in $BaBiO_3$ thin films on $SrTiO_3$
A19	Patrick Salg (*Technische Universität Darmstadt, Germany*) Oxygen diffusion in epitaxial oxide heterostructures with $SrMoO_3$ thin films
A20	Tornike Gagnidze (*EMPA, Switzerland*) Study of structural properties of ultrathin SrO films deposited on $SrTiO_3$
A21	Wolfgang Braun (*MPI Stuttgart, Germany*) Substrate Preparation and High-Temperature Stoichiometry Control of Oxide Surfaces
A22	Woo Jin Kim (*Institute for Basic Science, Republic of Korea*) The fine phase control of pyrochlore iridates epitaxial films using sequential pulsed annealing epitaxy
A23	Yeaju Jang (*Seoul National University, Republic of Korea*) Transparent thin film transistors of polycrystalline SnO_{2-x} and epitaxial SnO_{2-x}
A24	A. Vailionis (*Stanford University, USA*) Tuning Interfacial Ferromagnetism via Crystallographic Symmetry Mismatch
A25	B. Kim (*Seoul National University, Republic of Korea*) Robust 2D Skyrmions in ultra-thin $SrRuO_3$ film

A26	Changan Wang (*Helmholtz-Zentrum Dresden-Rossendorf, Germany*) Defect-induced exchange bias in a single $SrRuO_3$ layer
A27	Deepak Kumar (*University of Normandie, France*) Mechanical strain engineering of magnetism in $PrVO_3$ thin films
A28	G. Araizi-Kanoutas (*University of Amsterdam, The Netherlands*) What does and does not lie behind emergent thickness- dependent ferromagnetism in $LaMnO_3$ films
A29	Gennadii Laskin (*MPI Stuttgart, Germany*) $SrRuO_3$ as a Model System for Quantum Dots of Correlated Materials
A30	J.R. Hortensius (*Delft University of Technology, The Netherlands*) Ultrafast control of the Morin phase transition in the magnetic oxide $DyFeO_3$ by phonon pumping
A31	June Hyuk Lee (*Korea Atomic Energy Research Institute, Republic of Korea*) Polarised Neutron Reflectivity Study of Magnetic Oxides Thin Films using HANARO Reflectometers
A32	Lim Zhi Shiuh (*National University of Singapore, Singapore*) Ferrimagnetic Skyrmion in a Charge-transfer Superlattice
A33	Martina Müller (*University Duisburg-Essen, Germany*) Tailoring magnetic oxide quantum wells
A34	R. Aeschlimann (*CNRS, Thales, France*) Non-collinear magnetism and "living-dead" layer in rare earth titanate thin films
A35	Sergi Martín Rio (*ICMAB-CSIC, Spain*) Complex Oxide Heterostructures for Spin Electronics
A36	Xiaofang Zhai (*University of Science and Technology of China, China*) Strain-induced high-temperature perovskite ferromagnetic insulator
A37	Yingfen Wei (*University of Groningen, The Netherlands*) Magnetic tunnel junctions based on ferroelectric $Hf_{0.5}Zr_{0.5}O_2$ tunnel barriers
A38	Zhenping Wu (*Beijing University of Posts and Telecommunications, China*) Anomalous negative electroresistance and giant resistance modulation in epitaxial manganite/piezoelectric heterostructures
A39	Alla Chikina (*PSI, Switzerland*) Orbital ordering of the mobile and localizedelectrons at oxygen-deficient $LaAlO_3/SrTiO_3$ interfaces.
A40	Binbin Chen (*University of Twente, The Netherlands*) Interfacial octahedral coupling and dimensionality controlled electronic transitions in $NdNiO_3/SrTiO_3$ superlattices
A41	Jennifer Fowlie (*University of Geneva, Switzerland*) Exploring the phase diagram of $Nd_{1-x}La_xNiO_3$ thin films
A42	L.R. Viannie (*Indian Institute of Science, India*) Phase transition induced micromechanical actuation in VO_2 coated cantilever
A43	M. Souri (*University of Kentucky, USA*) Mott Variable-Range Hopping Transport in Sr_2IrO_4 Epitaxial Thin Films
A44	Q. Guo (*University of Groningen, The Netherlands*) Bad-metalicity and microstructure in rare-earth nickelates
A45	C. W. Schneider (*PSI, Switzerland*) Multiferroic properties of coherently grown orthorhombic $RMnO_3$ (R = Gd-Lu) thin films
A46	Daniele Preziosi (*University of Strasbourg, France*) Tailoring 'trapped' electrons in Ferroelectric Field Effect Devices
A47	Hahoon Lee (*Seoul National University, Republic of Korea*) Ferroelectric field effect transistor based on $BaSnO_3$
A48	Iaroslav Gaponenko (*University of Geneva, Switzerland*) Local and correlated studies of humidity-mediated ferroelectric thin film surface charge dynamics
A49	M. Viret (*CEA, France*) Imaging and modifying antiferromagnetic configurations in $BiFeO_3$
A50	Minh Thanh Do (*University of Twente, The Netherlands*) Ferroelectric fatigue of $PbZr_{0.52}Ti_{0.48}O_3$ epitaxial thin films: from cause and mechanism to strategies to avoid

A51	P. J. Ryan (*Argonne National Laboratory, USA*) Employing in-situ Frequency Dependent X-ray Scattering to Explore the Microscopic Response of Electrically Driven Epitaxial Strained and Free Membrane PMN-30PT thin films at the Morphotropic Phase Boundary.
A52	Pablo Vales (*ICN2, Spain*) Antiferroelectrics: flexoelectric and electrocaloric response
A53	Saúl Estandía (*ICMAB-CSIC, Spain*) Imaging Polarization Topologies in $BaTiO_3/SrTiO_3$ Superlattices
A54	Sungmin Park (*Seoul National University, Korea*) Selective control of multiple ferroelectric switching pathways using trailing flexoelectric field and its implications
A55	Vikas Shabadi (*Radiant Technologies, USA*) Advanced Functional Testing of Oxide Electronic Systems
A56	A.E.M Smink (*University of Twente, The Netherlands*) Direct tunneling and capacitance spectroscopy in Au - $(LaAlO_3)_4$ - $SrTiO_3$ tunnel junctions
A57	Alexander A. Demkov (*University of Texas, USA*) Large positive linear magnetoresistance in the two-dimensional t_{2g} electron gas at the $EuO/SrTiO_3$ interface
A58	J. Khmaladze (*University of Fribourg, Switzerland*) Coupled Cu- and Mn charge and orbital orders in cuprate/manganite
A59	Daseob Yoon (*Pohang University of Science and Technology, Republic of Korea*) Oxygen-vacancy-assisted recovery process for increasing electron mobility in n-type $BaSnO_3$ epitaxial thin films
A60	Eric N. Jin (*Yale University, USA*) 2-dimensional electron gas oxide remote doping of Si(001)
A61	F.Y. Bruno (*University of Geneva, Switzerland*) Two-Dimensional Electron Gases at the (111) - Surfaces of $KTaO_3$ and $SrTiO_3$
A62	Gervasi Herranz (*ICMAB-CSIC, Spain*) Photoresponse dynamics and photoconductivity mapping in $LaAlO_3/SrTiO_3$ interfaces
A63	Giordano Mattoni (*Delft University of Technology, The Netherlands*) Charge doping and large lattice expansion in oxygen-deficient heteroepitaxial WO_3
A64	J. Tornos (*Universidad Complutense de Madrid, Spain*) Ionic Liquid Gating of $SrIrO_3$ Ultra-Thin Films
A65	Jinkwon Kim (*Seoul National University, Republic of Korea*) The fabrication of s-wave/p-wave superconducting oxide heterojunctions
A66	Judith Gabel (*Universität Würzburg, Germany*) Interface band engineering in $LaAlO_3/SrTiO_3$ heterostructures
A67	M. Mirjolet (*ICMAB-CSIC, Spain*) Misfit Controlled Electrical Conductivity and Simultaneous Optimization of Carrier Density and Mobility in Transparent Metallic $3d$ Oxide Films
A68	M. von Soosten (*Technical University of Denmark, Denmark*) Seeing the birth of conductivity at oxide interfaces - an in-situ transport study
A69	N. Lebedev (*Leiden University, The Netherlands*) Inducing magnetism in the electron gas at $LaAlO_3/GdTiO_3/SrTiO_3$ interfaces
A70	Omar Ganesh Ji (*National University of Singapore*) The Effect of $LaFeO_3$ Spacer Layer on Electrical Properties of $LaAlO_3/SrTiO_3$ Interfaces
A71	P. Zhang (*University of Groningen, The Netherlands*) Unconventional anomalous Hall effect in $SrRuO_3$ thin films
A72	Ritsuko Eguchi (*University of Geneva, Switzerland*) Superconductivity at $LaAlO_3$/Ca doped $SrTiO_3$ interfaces
A73	S. W. Zeng (*National University of Singapore, Singapore*) Electrolyte gating on high-Tc cuprates: superconductor-insulator phase transition and mechanism investigation
A74	Sizhao Huang (*University of Twente, The Netherlands*) Strain induced polar metal in $(LaTiO_3)_n/(LaVO_3)_n$ superlattices
A75	T. Harada (*Tohoku University, Japan*) Nonlinear Hall effect originated from the surface of $PdCoO_2$ ultrathin films

A76	V.N. Strocov (*PSI, Switzerland*) **k**-resolved electronic structure of buried oxide and semiconductor interfaces explored by soft-X-ray ARPES
A77	Weiwei Luo (*University of Geneva, Switzerland*) Temperature dependent scanning near-field optical microscopy of $LaAlO_3/SrTiO_3$ interfaces
A78	Y. Z. Chen (*Technical University of Denmark, Denmark*) Scavenging of oxygen vacancies at modulation-doped oxide interfaces: Evidence from oxygen isotope tracing
A79	Yildiz Gozde Saglam (*Delft University of Technology, The Netherlands*) Probing the superconducting state of $SrTiO_3/LaAlO_3$ by superconducting coplanar waveguide resonators
A80	Yu Zhang (*Chinese Academy of Sciences, China*) Metallic Conduction and Ferromagnetism in $MAl_2O_4/SrTiO_3$ Spinel/Perovskite Heterostructures (M = Fe, Co, Ni)
A81	Alain Mercy (*University of Liège, Belgium*) Charge- versus orbital-order in e_g^1 perovskites
A82	Claude Ederer (*ETH Zurich, Switzerland*) The coupled structural and electronic metal-insulator transition in rare earth nickelates from DFT+DMFT
A83	Eric Bousquet (*University of Liège, Belgium*) First-principles study of ferroelectricity, antiferroelectricity and polarons in WO_3
A84	Philippe Ghosez (*University of Liège, Belgium*) Engineering large and reversible Rashba spin splitting in ferroelectric perovskite oxides and related compounds
A85	Sébastien Lemal (*University of Liège, Belgium*) First-principles study of $SrTiO_3(001)/LaAlO_3/SrTiO_3$ heterostructures
A86	Sohrab Ismail-Beigi (*Yale University, USA*) BoSS your oxide
A87	Xu He (*University of Liège, Belgium*) Toward a unified view on the metal-insulator transition in nickelates

Poster Session B

B1	C. Frontera (*ICMAB-CSIC, Spain*) Ferromagnetic insulating perovskite for nonvolatile memory device and anisotropic sensor
B2	Daniel M. Cunha (*University of Twente, The Netherlands*) Mapping Electrochemical Activity at the Nanoscale for Enhanced Solid-State Battery Electrodes
B3	J. G. Connell (*University of Kentucky, USA*) Hydrogen plasma induced Mott-insulating and transparent-conducting states in epitaxial $Ba_{0.5}Sr_{0.5}TiO_3$ thin-films
B4	L. Alff (*Technische Universität Darmstadt, Germany*) Atomically interface engineered micrometer-thick oxide electrodes for thin dielectrics tunable at ion battery voltage
B5	Y. Uzun (*University of Twente, The Netherlands*) Generation and detection of surface acoustic waves on strain-induced piezoelectric $SrTiO_3$
B6	Yunkyu Park (*Pohang University of Science and Technology, Republic of Korea*) Steep-slope NbO_2-based threshold switch enabled by pulsed-laser-induced phase transformation
B7	Adrian David (*University of Normandie, France*) Polycrystalline ceramics: a new generation of substrates using combinatorial epitaxy
B8	Amit Khare (*Indian Institute of Science, India*) Real-time observation of reversible topotactic phase transition in epitaxial $SrFeO_x$ thin films
B9	C.A.J. de Hond (*University of Twente, The Netherlands*) Atomic control of disorder in PZT and epitaxial integration on GaN for high-power devices
B10	Claudia Cancellieri (*EMPA, Switzerland*) Complex oxidation behavior of $W_xTi_{1-x}O_y$ alloys
B11	Dirk Fuchs (*Karlsruher Institut für Technologie, Germany*) Electronic transport in (110) $SrIrO_3$ heterostructures
B12	F.V.E. Hensling (*Forschungszentrum Juelich, Germany*) UV radiation enhanced oxygen vacancy formation caused by the PLD plasma plume
B13	Huan Ma (*EMPA, Switzerland*) Single-crystal Strontium Aluminate thin films by pulsed laser deposition
B14	Hyeongmin Cho (*Seoul National University, Republic of Korea*) Effect of $Ba_xSr_{1-x}HfO_3$ buffer layer on La-doped $BaSnO_3$
B15	Jeong Rae Kim (*Seoul National University, Republic of Korea*) Preparation of atomically flat, single terminated $LaAlO_3$ (001) substrate surfaces through thermal annealing and deionized water leaching
B16	Lukas Zeinar (*Technische Universität Darmstadt, Germany*) Effect of Ti stoichiometry on crystal and electronic structure of single crystalline epitaxial $Ba_{0.5}Sr_{0.5}Ti_{1+y}O_3$
B17	Nicola Manca (*Delft University of Technology, The Netherlands*) Understanding the semimetallic state of $SrIrO_3$ thin films: from epitaxial growth to thermal and magneto-transport studies
B18	T.P.P. Le (*University of Twente, The Netherlands*) Tailoring Vanadium Dioxide Thin Film Orientation by $Ti_{0.87}O_2$ and $NbWO_6$ Nanosheets
B19	Victor Fuentes (*ICMAB-CSIC, Spain*) Thickness dependence of electronic properties in $SrIrO_3$ thin films grown by sputtering
B20	Wolfgang Stein (*SURFACE systems+technology GmbH+Co, Germany*) Multi Process Thin Film Deposition and complex Sample Preparation Cycle under protected Atmosphere
B21	Y.F. Nie (*Nanjing University, China*) Realization of freestanding transition metal oxide 2D crystals of sub-nanometer thickness
B22	Yorick Birkhölzer (*University of Twente, The Netherlands*) Large area PLD of ferroelectric oxides on silicon for neuromorphic applications
B23	Alberto Pomar (*ICMAB-CSIC, Spain*) Magnetic anisotropy and spin dynamics in chemically deposited $La_{0.92}MnO_3$ thin films
B24	C. Leighton (*University of Minnesota, USA*) Giant Electrostatic Modification of Magnetism via Electrolyte-Gate-Induced Cluster Percolation in Epitaxial $La_{1-x}Sr_xCoO_3$

B25	D. Afanasiev (*Delft University of Technology, The Netherlands*) Resonant control of magnetism via selective excitation of the lattice vibration in magnetic oxide $DyFeO_3$
B26	F. Trier (*CNRS, Thales, France*) Non-local Detection of Spin diffusion in $LaAlO_3/SrTiO_3$ Heterostructures
B27	G. Bimashofer (*PSI, Switzerland*) Reversible magnetoelectric switching by electrochemical lithium intercalation
B28	Hiro Nakamura (*MPI Stuttgart, Germany*) Axial spin-momentum locking and valley degree of freedom in antiperovskite Dirac materials
B29	John Edward Ordoñez (*Universidad del Valle, Colombia*) Analysis of magnetic anisotropy on in artificially multiferroic $BaTiO_3/La_{2/3}Sr_{1/3}MnO_3$ heterostructures
B30	Lim Zhi Shiuh (*National University of Singapore, Singapore*) Paramagnetic to antiferromagnetic quantum critical phase transition induced by bandwidth reduction
B31	Marta Gibert (*University of Zurich, Switzerland*) Double-perovskite La_2NiMnO_6: a thin film and a superlattice approach
B32	P. Radhakrishnan (*MPI Stuttgart, Germany*) Structural and electronic properties of rare-earth vanadate heterostructures
B33	Ryan Need (*NIST, USA*) Controlling magnetization in $SrTiO_3$ quantum wells embedded within Mott insulating heterostructures
B34	T. Tybell (*Norwegian University of Science and Technology, Norway*) The role of atomic reconstructions and antiferromagnetic spin structure to establish emerging interface spin textures at the (111)-oriented $La_{0.7}Sr_{0.3}MnO_3/LaFeO_3$interface
B35	Xuefeng Wang (*Nanjing University, China*) Origin of Emergent Ferromagnetism in Otherwise Antiferromagnetic $LaMnO_3$ Thin Films
B36	Yichen Jia (*Yale University, USA*) Controllable Spin Injection across a Crystalline $BaTiO_3$-Germanium Interface
B37	Zhangzhang Cui (*University of Science and Technology of China, China*) Intrinsic magnetism of Aurivillius-type multiferroic thin films probed by resonant inelastic X-ray scattering and polarized neutron reflectivity
B38	C. Dominguez (*University of Geneva, Switzerland*) Electrical properties of $(111)_{pc}$ $SmNiO_3/NdNiO_3$ superlattices
B39	E. Cappelli (*University of Geneva, Switzerland*) Laser-ARPES Investigation of the Electronic Structure of $LaNiO_3$ Thin Films
B40	Katrin Fürsich (*MPI Stuttgart, Germany*) Ultrahigh-resolution Resonant Inelastic X-ray Scattering from rare-earth nickelates: magnetic and *dd*-excitations
B41	Sebastiaan van Dijken (*Aalto University School of Science, Finland*) In Situ TEM of Structural and Resistive Phase Transitions in $La_{2/3}Sr_{1/3}MnO_3$ Driven by Voltage Pulses and Strain
B42	C. Weymann (*University of Geneva, Switzerland*) Controlling defect distribution and intrinsic polarization state ultrathin ferroelectric films
B43	Dowon Song (*Seoul National University, Republic of Korea*) $BaHf_{1-x}Ti_xO_3$, high-k perovskite dielectric
B44	Hiroyasu Yamahara (*University of Tokyo, Japan*) Magnetic and Dielectric Properties of Strained Garnet Ferrite Thin Films
B45	Milena Cervo Sulzbach (*ICMAB-CSIC, Spain*) Thermionic Field Emission in back-to-back $BaTiO_3$-based Schottky interfaces

B46	Nagarajan Valanoor (*The University of New South Wales, Australia*) Non-volatile Ferroelectric Domain Wall Memory
B47	P. Tückmantel (*University of Geneva, Switzerland*) From local to macroscale switching dynamics in $Pb(Zr_{0.2}Ti_{0.8})O_3$ thin films
B48	Pu Yu (*Tsinghua University, China*) Magnetoelectric coupling through the electric-field controlled ionic evolution
B49	Rajesh Mandal (*Georg-August-Universität Göttingen, Germany*) Electrical and Magnetic Properties of Hexagonal $TbMnO_3$-based Heterostructures
B50	Shinhee Yun (*KAIST, Republic of Korea*) Flexoelectric polarizations at ferroelastic domain walls in non-ferroelectric WO_3 thin films
B51	Yinlian Zhu (*Chinese Academy of Sciences, China*) Giant polarization sustainability in ultrathin ferroelectric films characterized by Cs-corrected transmission electron microscopy
B52	A.E.M Smink (*University of Twente, The Netherlands*) Electrostatic control of the band structure and of superconductivity at the $LaAlO_3$-$SrTiO_3$ interface
B53	Ai Ikeda (*NTT Corporation, Japan*) Hole carriers driving superconductivity in infinite-layer cuprates
B54	Chunhai Yin (*Leiden University, The Netherlands*) Gate tunable carrier density and mobility at the $LaAlO_3/SrTiO_3$ interface
B55	Dennis Valbjørn Christensen (*Technical University of Denmark, Denmark*) Tuning the electronic and magnetic properties of γ-$Al_2O_3/SrTiO_3$
B56	Eric Teipel (*University of Kentucky, USA*) Observation of the topological Hall efect in $SrRuO_3$ thin-films
B57	Fabio La Mattina (*EMPA, Switzerland*) Angular Photoemission Spectroscopy investigation of STO/YBCO interface
B58	Gideok Kim (*MPI Stuttgart, Germany*) Cation substitution driven apical oxygen vacancies in overdoped La-214 cuprates and its superconducting properties
B59	Haichao Xu (*Fudan University, China*) Unveiling the superconducting mechanism of $Ba_{0.51}K_{0.49}BiO_3$
B60	Jiyeon Lee (*Univ. of Tokyo, Japan*) Magnetotransport at $SrTiO_3/LaTiO_3$ interfaces
B61	Kyeong Tae Kang (*Sungkyunkwan University,Reublic of Korea*) Examination of synergetic conductance in graphene-$SrTiO_3$ thin film heterostructure
B62	M. Uchida (*University of Tokyo, Japan*) Enhancement of Upper Critical Field in Superconducting Sr_2RuO_4 Thin Films
B63	Margherita Boselli (*University of Geneva, Switzerland*) Electronic transport in low dimensions: conducting nanowires at the $LaAlO_3/SrTiO_3$ interface
B64	N. Lebedev (*Leiden University, The Netherlands*) Presence of a hole band at the $LaTiO_3/SrTiO_3$ interface
B65	P. Reith (*University of Twente, The Netherlands*) Magnetic and electrical properties of combined $LaAlO_3$ and $LaMnO_3$ heterostructures on $SrTiO_3$
B66	K. Rubi (*LNCMI Toulouse, France*) Non 1/B-periodic Shubnikov-de Haas oscillations in gate tunable 2DEG at the $LaAlO_3/SrTiO_3$ interface
B67	S.A. Chambers (*Pacific Northwest National Laboratory, USA*) Layer-Resolved Band Bending at the n-$SrTiO_3(001)/p$-Ge(001) Interface
B68	Shengwei Zeng (*National University of Singapore, Singapore*) Searching for high-mobility two-dimensional electron gas at oxide interfaces through electrolyte gating
B69	Stephan Geprägs (*Bayerische Akademie der Wissenschaften, Germany*) Spin Hall magnetoresistance in antiferromagnet/heavy-metal heterostructures
B70	T.C. van Thiel (*Delft University of Technology, The Netherlands*) Interfacial anomalous Hall effects in ultrathin $LaAlO_3/SrRuO_3$ heterostructures

B71	Wei-Li Lee (*Academia Sinica, Taiwan*) Determination of Spin-Orbit Scattering Lifetime at the Interface of $LaAlO_3/SrTiO_3$ from the Superconducting Upper Critical Fields
B72	William M. Postiglione (*University of Minnesota, USA*) Electron Mobility Optimization in High-Pressure-Oxygen-Sputtered Epitaxial $Ba_{1x}La_xSnO_3$ Thin Films
B73	Y. L. Gan (*Technical University of Denmark, Denmark*) Tuning the Ground State of Oxide Interfaces by an Electron Sink
B74	Youjung Kim (*Seoul National University, Korea*) 2D-like $LaInO_3$ /$BaSnO_3$ polar interface on MgO substrate
B75	Alexandru B. Georgescu (*Flatiron Institute, USA*) Dimensionality Effects on the Metal-Insulator Transition in Nickelate Heterostructures
B76	Danila Amoroso (*University of Liège, Belgium*) First-principles study of (Ba,Ca)TiO_3 and Ba(Ti,Zr)O_3 solid solutions
B77	Pierre Bruneel (*Université Paris-Sud, France*) Topological phases of (111) oriented $LaAlO_3$-$SrTiO_3$ interfaces
B78	Shuai Dong (*Southeast University, China*) Appearance and disappearance of ferromagnetism in ultra-thin $LaMnO_3$ on $SrTiO_3$ substrate: a viewpoint from first-principles
B79	Wen-Yi Tong (*University of Liège, Belgium*) First-principles modeling for $SrTiO_3$/Si interfaces
B80	Daisuke Kan (*Kyoto University, Japan*) Anomalous behavior in transverse resistivity in the itinerant ferromagnetic oxide $SrRuO_3$

Single spin magnetic sensing of mesoscopic condensed matter systems

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Electronic spins yield excellent quantum sensors [1], offering quantitative sensing [2] and nanoscale imaging [3] down to the level of single spins [4]. Over the last years, the Basel Quantum Sensing Group has developed all-diamond scanning probes [5,6], hosting individual Nitrogen-Vacancy (NV) centre electronic spins as nanoscale magnetometers, to address open problems in condensed matter physics. I will describe our recent advances in applying this novel and unique quantum-sensing technology to study nano-magnetism at room temperature as well as mesoscopic systems in cryogenic environments down to the millikelvin range.
Specifically, I will discuss applications of NV magnetometry in the emerging field of antiferromagnetic spintronics [7], where our quantum sensors can address thin-film antiferromagnets with unprecedented performance to reveal nanoscale domains [8] and non-trivial spin-textures [9]. The robustness of our scanning NV magnetometers further allows for their use under cryogenic conditions [10], where I will highlight recent advances in studying electron transport in two-dimensional systems such as graphene or oxide interfaces.

[1] B. Chernobrod and G. Berman, Journal of Applied Physics **97**, 014903 (2004)
[2] J. Taylor *et al.*, Nature Physics **4**, 810 (2008)
[3] L Rondin *et al.*, Rep. Prog. Phys. **77**, 056503 (2014)
[4] M. S. Grinolds *et al.*, Nature Physics **9**, 215 (2013)
[5] P. Appel *et al.*, Review of Scientific Instruments **87**, 063703 (2016)
[6] P. Maletinsky *et al.*, Nature Nanotechnology **7**, 320 (2012)
[7] T. Jungwirth *et al.*, Nature Nanotechnology **11**, 231 (2016)
[8] T. Kosub *et al.*, Nature Communications **8**, 13985 (2017)
[9] I. Gross *et al.*, Nature **549**, 252 (2017)
[10] L. Thiel *et al.*, Nature Nanotechnology **11**, 677 (2016)

Light-induced symmetry breaking in $SrTiO_3$

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Selectively exciting collective modes in solids provides a means to control electronic behavior using light. For instance, resonantly driving optical phonons in complex oxide systems can induce ultrafast insulator-metal transitions or transient superconductivity at high temperatures. We use a similar approach to create a light-induced ferroelectric-like state in single crystal $SrTiO_3$. In equilibrium, $SrTiO_3$ remains centrosymmetric and paraelectric at all temperatures. By pumping the high-frequency optical phonon in $SrTiO_3$ with femtosecond light pulses, we find that an unusual long-lived state develops with broken centrosymmetry. Second harmonic imaging and polarimetry reveal that the light-induced state has a polar crystal symmetry with a pump-frequency dependent ferroelectric-like polarization. Time-resolved second harmonic generation points to a symmetry breaking mechanism resulting from nonlinear phonon-strain coupling. The polar state has a lifetime on the order of 10^3 seconds and can be erased by above gap excitation. The induced state is also found to generate sizeable short-circuit photocurrents upon excitation, providing a unique and technologically interesting platform for mid-infrared optoelectronic and photovoltaic applications which may integrated with functional oxide films.

Breaking not-so-bad: fracture flexoelectricity

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Flexoelectric polarization has mechanical consequences. Flexoelectricity is generated by strain gradients, and these are largest at the fracture fronts of propagating cracks. Fracture fronts thus generate flexoelectric fields that have an energy cost which, in turn, affects the mechanical properties of materials. In ferroelectrics, this cost depends on the ferroelectric polarity, meaning that one can change the mechanical response of a ferroelectric by switching its polarization -or, perhaps usefuly, use the mechanical response in order to "read" the polarity of a ferroelectric without having to use electrodes. Interestingly, the polarity dependence of fracture properties also means that crack propagation can be promoted or mitigated with a voltage, something that might have practical consequences with regards electromechanical fatigue of piezoelectric actuators.

Another quirck of crack-generated flexoelectricity is that it appears to have profound consequences even for our own survival as vertebrates. We have measured the bending-induced polarization of bones and bone mineral (hydroxyapatite), finding them to be of the same order of magnitude (around 1nC/m), which implies that hydroxyapatite flexoelectricity, and not collagen piezoelectricity, dominates electromechanical response of bone to local deformations. Among the deformations that happen in bones are fractures -including micro-fractures that are ubiquitous even in healthy bone. Using our measured flexoelectric coefficients of hydroxyapatite, we have calculated the flexoelectric fields generated around bone cracks, and discovered that they are large enough to cause apoptosis (programmed cell death) of osteocites, which is the known first step of bone healing. Flexoelectricity thus appears to be a principal actor in the process by which our bones heal themselves.

[1] K. Cordero, N. Domingo, A. Abdollahi, J. Sort, G. Catalan, Ferroelectrics as Smart Mechanical Materials, Advanced Materials 29, 1702210 (2017).

[2] F. Vasquez-Sancho, A. Abdollahi, D. Damjanovic, G. Catalan. Flexoelectricity in bones. Advanced Materials. 1705316 (2018).

Ferroelectricity in 1D Tetrahedral Chain Network via Combined Polar Distortion

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Recent advances in engineering transition metal-oxygen (TMO) octahedra led to a fundamental understanding on the functionalities emerging at transition metal oxides. Unconventional ferroelectricity can also emerge as a consequence of a collective distortion of TMO_6 octahedra in two dimensional networks. In the meantime, TMO_x polyhedra with different oxygen coordinate, such as TMO_4 tetrahedra with a lower structural symmetry can also form a low dimensional network and can exhibit intuitive inversion symmetry breaking through a collective distortion. In this talk, we focus on brownmillerite strontium ferrite $SrFeO_{2.5}$ (SFO). The brownmillerite structure possesses one-dimensionally ordered oxygen vacancy channels, which can equivalently be viewed as a one-dimensional chain of FeO_4 tetrahedra. Furthermore, a collective rotation of the FeO_4 tetrahedra, or a combined polar distortion, can break the structural inversion symmetry, which can be observed from the imaginary phonon dispersion at both zone-center and zone-boundary. The ferroelectricity expected in 1D tetrahedral network, is experimentally validated by second harmonic generation, piezoforce microscopy, and switching current measurements. Based on the inversion symmetry, possible correlation to the magnetic ordering will be also discussed.

Connecting ferroelectricity and superconductivity in $SrTiO_3$

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Perovskite-structure strontium titanate is a versatile and intriguing material, with diverse properties ranging from unconventional superconductivity to giant dielectric response associated with quantum paraelectricity. Here we argue that these behaviors are likely related, by proposing the ferroelectric quantum fluctuations as the source of the superconductivity. Using density functional calculations of the ferroelectric soft mode frequency in $SrTiO_3$ as a function of doping, we demonstrate a crossover related to quantum paraelectricity at a doping level coincident with the experimentally observed top of the superconducting dome. Based on this observation, we suggest a model in which the ferroelectric soft mode fluctuations provide the pairing interaction for superconductivity. Within our model, the low doping limit of the superconducting dome is explained by the emergence of the Fermi surface, and the high doping limit by departure from the quantum critical regime. We predict, using strong coupling theory within this framework of quantum criticality, that the highest critical temperature will increase and shift to lower carrier doping with increasing ^{18}O isotope substitution as well as with strain, and provide the first experimental hints verifying our prediction. Finally, we introduce the concept of multiferroic quantum criticality, propose materials related to $SrTiO_3$ in which it should occur, and describe the unconventional scalings of susceptibilities that will provide signatures of its existence.

Superfluid stiffness in oxide interfaces

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The discovery of a gate-tunable 2D superconducting electron gas [1] in oxide hetero-interfaces in coexistence with both ferromagnetism [2] and a strong Rashba spin-orbit coupling [3], has raised a considerable interest. However, the evolution of fundamental parameters with electrostatic doping, such as the pairing strength between electrons (i.e. the gap energy Δ) is non trivial [4]. We will present recent resonant microwave transport measurements on LaAlO3/SrTiO3 interfaces that allows extracting the superfluid stiffness Js, i.e. the energy scale which determines the cost of a phase twist in the superconducting condensate. We find that the competition between Js and Δ controls the superconducting phase diagram obtained by plotting the superconducting Tc as a function of gate voltage. Whereas a good agreement with the Bardeen-Cooper-Schrieffer (BCS) theory is observed at high carrier doping, our data suggest that the suppression of Tc at low doping is controlled by the loss of macroscopic phase coherence instead of electron pairing as in standard BCS theory. The analysis of the superfluid density also reveals that only a very small fraction of the electrons condenses into the superconducting state, which we relate to the filling of specific orbitals in the interfacial quantum well [5].

[1] A. D. Caviglia et al. Nature 456, 624 (2008).
[2] J. Bert et al. Nature Phys. 7, 767771 (2011).
[3] A. D. Caviglia et al. Phys. Rev. Lett. 104, 126803 (2010).
[4] C. Richter et al. Nature 502, 528531 (2013)
[5] G. Singh et al, Nat. Commun. 9, 407 (2018).

Enhanced spin-to-charge conversion through topological states in $SrTiO_3$-based two-dimensional electron gases

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The quasi 2D electron system (q2DES) that forms at the surface of $SrTiO_3$ (STO) capped with an ultrathin metallic layer is starting to gain attention from the oxide electronics community [1,2]. Unlike for the celebrated LAO/STO system, this approach allows the formation of a q2DEG through the deposition of a simple metal at room-temperature, and the q2DEG properties can be dramatically tuned depending on the metal used. Additionally, just like for LAO/STO [3], the Rashba spin-orbit coupling present at the STO surface may be exploited to interconvert spin and charge currents through the direct and inverse Edelstein effect, which presents exciting advantages for future spintronic devices [4,5].
In this presentation, we will show experiments performed on the q2DES formed in NiFe/(metal)/STO heterostructures. We investigate the nature of the inverse Edelstein effect (responsible for the spin-to-charge conversion) through a combination of spin pumping, magnetotransport, XPS, ARPES and theory. In particular, we will explore the highly-doped regime where topological states have been predicted at special points in the band structure [6]. There, spin-charge conversion should reach extremely high values.

[1] T. C. Rödel et al., Adv. Mater. 28, 1976 (2016)
[2] D. C. Vaz et al., Adv. Mater. 29, 1700486 (2017)
[3] E. Lesne, D.C. Vaz et al., Nat. Mater. 15, 1261 (2016)
[4] J. Varignon et al., Nat. Phys. 14, 322 (2018)
[5] S. Manipatruni et al., Nat. Phys. 14, 338 (2018)
[6] M. Vivek et al., Phys. Rev. B 95, 165117 (2017)

Revealing the role of the interface in the high-temperature superconductivity of single-layer FeSe/$SrTiO_3$

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At the interface between monolayer FeSe films and $SrTiO_3$ substrate the superconducting transition temperature (T_c) is unexpectedly high, triggering a surge of excitement. The mechanism for the T_c enhancement has been the central question, as it may present a new strategy for searching for higher T_c materials. To reveal this enigmatic mechanism, by combining advances in interfacial engineering, ARPES studies and extensive data from other techniques, we reveal how the superconductivity is related with various interfacial interactions. Our results point to the fascinating prospect that cooperation between different Cooper pairing channels may be a general framework to understand and design high-temperature superconductors.

In-situ strain-tuning of the metal-insulator-transition of Ca_2RuO_4 in angle-resolved photoemission experiments

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We report the evolution of the k-space electronic structure of lightly doped bulk Ca_2RuO_4 with uniaxial strain.Using ultrathin plate-like crystals, we achieve strain levels up to -4.1%, sufficient to suppress the Mott phase and access the previously unexplored metallic state at low temperature. Angle-resolved photoemission experiments performed while tuning the uniaxial strain reveal that metallicity emerges from a marked redistribution of charge within the Ru t_{2g} shell, accompanied by a sudden collapse of the spectral weight in the lower Hubbard band and the emergence of a well defined Fermi surface which is devoid of pseudogaps. Our results open new perspectives for spectroscopic measurements and suggest that lightly doped Ca_2RuO_4 has potential as active layer in piezoelectronic transistors.

Electron-lattice coupling in correlated electron materials: Ca_2RuO_4 and beyond

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'Mott' metal-insulator transition materials are commonly defined as compounds exhibiting an electronically driven metal to insulator transition. However, in many cases a lattice distortion is empirically known to occur simultaneously with the transition, and lattice energetics are important. This talk will examine these issues in the context of Ca_2RuO_4, which undergoes a metal-insulator transition that is coincident with a ferro-orbital ordering and exhibits a stron pressure dependence. A theory of the coupling of the metal-insulator transition to the lattice will be presented, remarkable implications for the dependence of the metal-insulator transition on epitaxial strain will be demonstrated, and a strain-induced multscale structure of domain walls separating insulating and metallic phases will be shown. Generalizations of the theory and extensions to other materials will be presented.

[1] Lattice Energetics and Correlation-Driven Metal-Insulator Transitions: the Case of Ca2RuO4, Q. Han and A. J. Millis, arXiv:1801:06215

Real-time observation of polarization emergence in ultrathin ferroelectric oxide heterostructures

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The integration of functional properties into oxide multilayer architectures demands for atomic precision. The conventional optimization process requires multiple samples and *ex-situ* analysis while *in-situ* diagnostic tools guarantee high structural quality but are usually
insensitive to the functionality targeted with the actual deposition. Here, we take advantage of the non-invasive nature of optical probes to monitor the intended functionality during growth.
Taking ferroelectricity as a representative case, we show that optical *in-situ* second harmonic generation (ISHG) analysis can be performed simultaneous to the pulsed-laser-deposition growth operation. We follow the evolution of the spontaneous polarization in real time and with monolayer resolution throughout the deposition process [1]. Such direct access allows validating the growth of oxide heterostructures with an arbitrary sequence of up- and down-polarized ferroelectric layers.
This is only the first step in the implementation of ISHG as a growth diagnostic tool. The *in-situ* access to emerging properties enables an unprecedented degree of control that can promote the engineering of oxides functionalities to a completely new level.

[1] G. De Luca *et al.*, Nat. Commun. **8**, 1419 (2017)

Topological Transitions in Ultrathin Ferroelectric Films

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I will present results of research on topological transitions in ultrathin epitaxial ferroelectric films. Observation of a new type of nanoscale ferroelectric domains, termed as "bubble domains", - laterally confined spheroids of sub-10 nm size with local dipoles self-aligned in a direction opposite to the macroscopic polarization of a surrounding ferroelectric matrix is reported. The bubble domains appear in ultrathin epitaxial $PbZr_{0.2}Ti_{0.8}O_3/SrTiO_3/PbZr_{0.2}Ti_{0.8}O_3$ ferroelectric sandwich structures due to the interplay between charge and lattice degrees of freedom. The existence of the bubble domains is revealed by high-resolution piezoresponse force microscopy (PFM), and is corroborated by aberration-corrected atomic-resolution scanning transmission electron microscopy mapping of the polarization displacements. An incommensurate phase and symmetry breaking is found within these domains resulting in local polarization rotation and hence impart a mixed Néel-Bloch-like character to the bubble domain walls. PFM hysteresis loops for the bubble domains reveal that they undergo an irreversible phase transition to cylindrical domains under the electric field, accompanied by a transient rise in the electromechanical response. Our observations are in agreement with ab-initio-based calculations, which reveal a very narrow window of electrical and elastic parameters that allow the existence of bubble domains. The findings highlight the richness of polar topologies possible in ultrathin ferroelectric structures and bring forward the prospect of emergent functionalities due to topological transitions.
The research is a collaboration between UNSW Sydney, U Arkansas, U Nebraska, Nanjing University and UC Irvine. This work appears in Zhang et al, Adv. Mater. 2017, 29, 1702375

[1] Adv. Mater. 2017, 29, 1702375

Electron microscopy study of the Metal-Insulator Transition in nickelate superlattices

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Rare-earth nickelate perovskites $ANiO_3$ possess a metal-insulator transition (MIT) that is tuneable in the bulk by the size of the rare-earth at the perovskite A site which influences the rotation of the NiO_6 octahedra.[1] In thin-film heterostructures, the rotation patterns can be altered by epitaxial strain. In this talk, we will present recent results that show that the oxygen octahedra rotations of a given compound can be precisely adjusted within a broad range by combining $SmNiO_3$ with a different perovskite used as a tilt-control layer (TCL). Through scanning transmission electron microscopy (STEM), the oxygen octahedral can be visualized and measured unit cell by unit cell.[2,3] We reveal a link at the atomic-scale between a decrease of the NiO_6 tilt angles and a reduced MIT temperature, further confirmed from a simple theoretical model.[4] In a second example using $RNiO_3$ (R=Sm, Nd) superlattices, we will demonstrate the relationship between metal-oxygen hybridization, oxygen octahedral tilt and metal-insulator transition in a similar way as we previously demonstrated for magnetism in STO buffered/unbuffered $La_{0.6}Sr_{0.4}MnO_3$ films deposited on $NdGaO_3$.[5]

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[1] J. Varignon, M.N. Grisolia, et al., Npj Quantum Mater. 2, 21 (2017)
[2] Z. Liao, M. Huijben, Z. Zhong, N. Gauquelin, et al., Nat. Mater. 15, 425 (2016)
[3] N. Gauquelin, K.H.W. van den Bos, et al., Ultramicroscopy 181, 178 (2017)
[4] Z. Liao, N. Gauquelin, et al., submitted (2018)
[5] Z. Liao, N. Gauquelin, et al., Adv. Funct. Mater. 27, 1 (2017)

Direct electromagnetic field imaging of interfaces by advanced STEM

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Due to the rapid progresses in segmented/pixelated detector developments in scanning transmission electron microscopy (STEM), differential phase contrast (DPC) imaging is becoming very powerful method to directly visualize electromagnetic field structures within materials and devices. It has been demonstrated that we can directly visualize atomic electric field, the field between positively charged atomic nucleus and negatively charged surrounding electron clouds [1-3] by using atomic-resolution DPC STEM. Fig. 1 show simultaneous (left) annular dark field (ADF) image, (center) electric field vector color map and (right) electric field strength map of $SrTiO_3$ crystal observed along [001] direction constructed from DPC STEM [3]. The direction of rotating color contrast is the same in all the atomic columns irrespective of the atomic species, visualizing that the (projected) atomic electric field points outward from the center of the atomic columns. In this talk, the current status of aberration-corrected DPC STEM along with some applications in materials studies such as pn junction in semiconductor devices and magnetic skyrmion in helimagnets [4] will be reported. New developments for atomic-resolution DPC STEM under magnetic field free condition will be also reported.

Fig. 1: (left) ADF image. (center) Projected electric field vector color map and (right) electric field strength map constructed from the segmented detector DPC images [3]. The inset color wheel indicates how color and shade denote the electric field orientation and strength in the vector color map.

[1] N. Shibata et al., Nature Phys., 8, 611-615 (2012).
[2] K. Müller et al., Nature. Comm. 5, 5653 (2014).
[3] N. Shibata et al., Nature Comm. 8, 15631 (2017).
[4] N. Shibata et al., Acc. Chem. Res., 50, 1502-1512 (2017).

Maximal Rashba-like spin splittings and intrinsic Stoner instabilities at polar surfaces of delafossite oxides

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The ABO_2 family of delafossite oxide metals host a rich array of bulk materials properties, ranging from ultra-high conductivity to unconventional magnetism [1,2]. I will discuss our angle-resolved photoemission (ARPES) studies of the surface electronic structure of the delafossite oxides (Pd,Pt)(Co,Rh)O_2. I will show how a surface polarity triggers a pronounced electron or hole doping, transforming the system from a single-band non-magnetic nearly-free electron metal in the bulk [3] to an itinerant ferromagnet with strong electron-magnon coupling [4], or to a correlated metal hosting a kinetic-energy-coupled inversion symmetry breaking [5] at their surfaces. The latter maximizes the influence of spin-orbit coupling, allowing this oxide surface to develop some of the largest Rashba-like spin splittings that are known.
Key collaborators on this work include Veronika Sunko (St Andrews and Max-Planck Institute for Chemical Physics of Solids, Dresden), Federico Mazzola (StA), and Helge Rosner, Pallavi Kushwaha, Seunghyum Khim, and Andy Mackenzie (MPI-CPFS).

[1] Ok *et al.*, Phys. Rev. Lett. **111** (2013) 176405
[2] Mackenzie, Rep. Prog. Phys. **80** (2017) 032501
[3] Kushwaha, Sunko*et al.*, Science Advances **1** (2015) e1500692
[4] Mazzola *et al.*, arXiv:1710.05392 (2017)
[5] Sunko *et al.*, Nature **549** (2017) 492

A theoretical investigation of graphene on a polar $SrTiO_3$ (111) surface

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Doping graphene layers presents a difficult practical and fundamental problem. We consider theoretically, the possibility of electrostatic doping of graphene by the intrinsic field of a polar substrate. By way of example, we perform density functional theory calculations for a graphene sheet placed on the (111)-oriented perovskite $SrTiO_3$ surface. We find that the Fermi surface moves well below the Dirac point of graphene, resulting simultaneously in a fast conducting channel in graphene, and a slow (large-effective-mass) channel at the oxide surface. Additionally, electrostatic gating may open a way to explore peculiar states that, through the "no-crossing", represent a hybrid carrier that exists simultaneously in both materials [1]. Moreover, further theoretical analysis suggests that coupling of electrons in graphene to interfacial hybrid plasmon/optical modes may result in effective attractive electron-electron interaction that, in turn, could result in electron pairing and lead to superconductivity.

[1] D. Shin and A. A. Demkov, "Theoretical investigation of the band alignment of graphene on a polar $SrTiO_3$ (111) surface", Phys. Rev. B **97**, 075423 (2018).

Orbital reconstruction and spin polarization in (100) and (111) LAO/STO and LAO/ETO/STO q2DEG

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In the last decade, the tremendous advances in the atomic-scale deposition of transition metal oxides have led to the discovery of novel functional electronic and magnetic properties at the oxide interfaces. One of the most important example is the discovery of a quasi-two-dimensional electron gas (q2DEG) at the interface between (001) SrTiO3 (STO) single crystals and LaAlO3 (LAO) [1].
Some of the distinctive properties of the (001) LAO/STO system arise from the occurrence of an orbital reconstruction, first demonstrated by x-ray linear dichroism (XLD) [2] and later on by Angle Resolved Photoemission Spectroscopy (ARPES) [3]. The orbital reconstruction causes a reverse ordering and splitting of the bulk conduction bands derived by non-degenerate t2g (3dxy, 3dxz, 3dyz) orbitals of Ti3d-states with D4h (tetragonal) crystal field. A similar orbital reconstruction is observed in delta doped (001) LAO/ETO/STO heterostructures, which have the interesting property to form a q2DEG characterized by a superconducting ground state and a spin-polarization [4].
In this talk I will present an overview of the electronic and magnetic properties of both (001) and (111) LAO/STO and LAO/ETO/STO q2DEG as investigated by x-ray spectroscopy, including x-ray absorption spectroscopy, x-ray linear and magnetic dichroisms. The results are compared to transport and magneto-transport properties of the system.

[1] Ohtomo and H. Y. Hwang, Nature 427, 423 (2004).
[2] M. Salluzzo, et al., Phys. Rev. Lett. 102, 166804 (2009).
[3] A. F. Santander-Syro, et al., Nature 469, 189 (2010).
[4] [1] D. Stornaiuolo, Nature Materials 15, 278-283 (2016).

Ferromagnetism and quantum anomalous Hall state in $SrRuO_3$ (111)

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$SrRuO_3$ is a promising candidate for thin film ferromagnetism, but heterostructures grown in the (001) direction time and again turned out to be non-magnetic below a critical thickness. By means of density functional theory (DFT) plus dynamical mean field theory (DMFT) [1], we show that for $SrRuO_3$ (111) instead a half-metallic ferromagnetic state with an ordered magnetic moment of 2 μB/Ru survives the ultimate dimensional confinement down to a bilayer, even at elevated temperatures of 500 K. In the minority channel, the spin-orbit coupling opens a gap at the linear band crossing corresponding to 3/4 filling of the t_{2g} shell. We predict that the emergent phase is Haldane's quantum anomalous Hall state with Chern number C=1, without any external magnetic field or magnetic impurities [2]. Similar physics with an even larger gap is also observed in $SrRhO_3$ (111) but not in $LaNiO_3$ (111) [3] bilayers.

[1] O. Janson, Z. Zhong, G. Sangiovanni, and K. Held, Dynamical mean field theory for oxide heterostructures, in Spectroscopy for Complex Oxide Interfaces, Eds: C. Cancellieri and V.N. Strocov, Springer (2018) [arXiv:1611.09044]
[2] L. Si, O. Janson, G. Li, Z. Zhong, Z. Liao, G. Koster, and K. Held, Phys. Rev. Lett. **119**, 026402 (2017).
[3] O. Janson and K. Held, arXiv:1804.00904.

Antiferroelectric $PbZrO_3$ Thin Film with multiple phase transitions

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Antiferroelectric (AFE) materials have attracted increasing attention for their potential applications in high-energy capacitors, high-strain actuators, IR pyroelectric detectors, and solid-state cooling devices, due to a remarkable and sharp change in polarization and volume during antiferroelectric to ferroelectric (FE) phase transition process. $PbZrO_3$ (PZO) is one of the first materials experimentally identified as antiferroelectric, as well as the end member in the most technologically used ferroelectric solid solution, lead zirconate titante. Many other PZO-based AFE materials share the same orthorhombic structure at room temperature, and hence understanding this material can further enhance our knowledge of a wide group of materials. However, processing of PZO films has been historically very challenging, and often has required various levels of doping to stabilize the antiferroelectric behavior and enhanced the properties.

Here we report on low-cost, chemical solution processed PZO thin films, deposited on platinized silicon substrates. The films' thickness was between 200 and 300 nm, with strong 002 and/or 042 crystallographic orientations (orthorhombic reference). No secondary phases were observed. This talk will specifically discuss the effects of processing parameters and doping on the microstructure of the films, the strength of the electric field for antiferroelectric-ferroelectric transitions, appearance of further ferroelectric transitions and the fundamental functional response. We will show that dielectric tunabilities over 88% and effective, and longitudinal piezoelectric coefficients, d_{33}, of approximately 700 to 1100 pm/V can be obtained through control of these processing parameters.

A high Li-ion conductivity atSolid-electrolyte and Electrode Interfaces: Introducing Oxide Epitaxial Thin-Film Technologyto Battery Research

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Solid-state Li batteries are promising energy-storage devices owing to their high-energy densities with improved safety. However, the large interface resistance at the interface of solid-electrolytes and electrodes hinders the development of the solid-state Li batteries.

Our group has been investigating surfaces and interfaces of transition-metal oxides, such as $SrTiO_3$, $LaAlO_3/SrTiO_3$, $SrVO_3$, $La_{0.7}Ca_{0.3}MnO_3$, and $LiTi_2O_4$, using epitaxial thin film deposition technology and scanning tunneling microscopy.[1)]

Here, we introduced the knowledge of oxide epitaxial thin films and oxide surfaces into battery research. We succeeded in fabricating the interface resistance below 5 Ωcm^2 ($Li_3PO_4/LiCoO_2$interface); the value is smaller than that of liquid-electrolyte-based Li-ion batteries.[2)]

We further introduce oxide thin film technology to solid-state nano-ionics; ionic diffusion is controlled by the epitaxial layer of a thickness less than 1 nm.

These studies strongly encourage solid-state Li battery research, by demonstrating a very low interface resistance leading to the fast charging and discharging.

[1] Hitosugi et al., ACS Nano, 5, 7967 (2011); Phys. Rev. Lett. 111, 126104 (2013); ACS Nano, 8, 2223 (2014); J. Am. Chem. Soc. 136, 17201 (2014); ACS Nano 9, 8766 (2015); Phys. Rev. Lett. 119, 086801 (2017); Nature Commun. 8, 15975 (2017).

[2] Hitosugi et al., Nano Lett. 15, 1498-1502 (2015).

All-oxide IR devices based on high-mobility CdO thin films

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Transparent conductive oxides (TCOs) are an attractive materials platform for plasmonics and metamaterials in the near- and mid-infrared (MIR). Among TCOs, doped cadmium oxide (CdO) exhibits exceptional electronic and plasmonic characteristics with tunable carrier concentration and high electron mobility, which enables low-loss plasmonic resonances. We have shown that through careful control of thin film growth and doping, doped CdO supports high quality plasmonic resonances across the entire MIR with tunable carrier concentrations spanning nearly than two orders of magnitude ($8x10^{19}$ to $4x10^{20}$ e^-/cm^3), accompanied by maximum carrier mobilities over 500 $cm^2/V{\cdot}s$. In the first part of the presentation we will show how high-intensity pulsed DC magentron sputtering from a Cd metal target can be used to grow epitaxial layers and CdO-CdO homojunctions in highly oxidizing gas atmospheres. In this growth mode, we simultaneously RF sputter a dopant cation to control carrier density.
In the second part of this talk, we will show that by controlling electron concentration, mobility, thickness, and film-substrate geometry, we can grow doped CdO films to engineer the IR optical response, and target multiple plasmonic modes, including surface plasmon polaritons (SPP), epsilon-near-zero (ENZ) modes, and Brewster/Berreman modes. Additionally, by growing stacked doped/intrinsic/doped CdO layers we are able to access additional SPP dispersion branches below the lightline resulting from coupling between the doped layers.
Such control further allows us to grow multilayer CdO films with arbitrary layer thickness and doping: in a single stack, we achieve multiple absorption peaks associated with the ENZ modes of each individual layers. In so doing, we can engineer light-matter interaction through the IR spectrum, manipulating both spectral absorption and emission. Finally, we will demonstrate how these efficient plasmonic absorbers can be used in conjuction with a rectifying schottky barrier or metal-insulator-metal tunnel junction to make a room temperature IR sensor based on internal photoemission of hot electrons that is tunable withing the IR spectrum.

Nature of the metal-insulator transition in few-unit-cell-thick $LaNiO_3$ films

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The nature of the metal insulator transition in thin films and superlattices of $LaNiO_3$ with only few unit cells in thickness remains elusive despite tremendous effort. Quantum confinement and epitaxial strain have been evoked as the mechanisms, although other factors such as growth-induced disorder, cation non-stoichiometry, oxygen vacancies, and substrate-film interface quality may also affect the observable properties in the ultrathin films. Here we report results obtained for near-ideal $LaNiO_3$ films with different thicknesses and terminations grown by atomic layer-by-layer laser molecular beam epitaxy on $LaAlO_3$ substrates. We find that the room-temperature metallic behavior persists until the film thickness is reduced to an unprecedentedly small 1.5 unit cells (NiO_2 termination). Electronic structure measurements using X-ray absorption spectroscopy and first-principles calculation suggest that oxygen vacancies existing in the films also contribute to the metal insulator transition.

Tailoring Materials for Mottronics: Excess Oxygen Doping of a Prototypical Mott Insulator

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The Mott transistor is a paradigm for a new class of electronic devices-often referred to by the term Mottronics-which are based on charge correlations between the electrons.[1,2] Since correlation-induced insulating phases of most oxide compounds are usually very robust, new methods have to be developed to push such materials right to the boundary to the metallic phase in order to enable the metal-insulator transition to be switched by electric gating.[3,4]

Here we demonstrate that thin films of the prototypical Mott insulator $LaTiO_3$ grown by pulsed laser deposition under oxygen atmosphere are readily tuned by excess oxygen doping across the line of the band-filling controlled Mott transition in the electronic phase diagram.[5] The detected insulator to metal transition is characterized by a strong change in resistivity of several orders of magnitude. The use of suitable substrates and capping layers to inhibit oxygen diffusion facilitates full control of the oxygen content and renders the films stable against exposure to ambient conditions. These achievements represent a significant advancement in control and tuning of the electronic properties of $LaTiO_{3+x}$ thin films making it a promising channel material in future Mottronic devices.

[1] H. Takagi, H. Y. Hwang, Science 2010, 327, 1601

[2] C. H. Ahn, J.-M. Triscone, J. Mannhart, Nature 2003, 424, 1015

[3] G. Mazza, A. Amaricci, M. Capone, M. Fabrizio, Phys. Rev. Lett. 2016, 117, 176401

[4] Z. Zhong, M. Wallerberger, J. M. Tomczak, C. Taranto, N. Parragh, A. Toschi, G. Sangiovanni, K. Held, Phys. Rev. Lett. 2015, 114, 246401

[5] P. Scheiderer, M.Schmitt, J. Gabel, M. Zapf, M. Stübinger, P.Schütz, L. Dudy, C. Schlueter, T.-L. Lee, M.Sing, and R. Claessen, Adv. Mater 2018, 1706708

Metal-Insulator Transition in Thin Films and Multilayers of Early Transition Metal Oxides from DFT+DMFT

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The wide variety of interesting phenomena and emerging functionalities observed in complex oxide thin films and heterostructures can be controlled by a large number of different factors, such as, e.g., substrate-induced epitaxial strain, dimensional confinement, interface-related effects, or defects. Here, we study the interplay between these effects in thin films and multilayers composed of different early transition metal oxides, including correlated metals, Mott insulators and band insulators, using a combination of density functional theory (DFT) and dynamical mean-field theory (DMFT).
We discuss several examples where these factors lead to modifications of structural as well as electronic properties, resulting in metal-insulator transitions. For instance, we investigate charge transfer due to potential gradients in polar heterostructures, the evolution of octahedral rotations across an oxide-oxide interface between two materials with different rotation angles and/or tilt systems, and how this affects the range of electronic reconstruction in the interfacial region. We show how these effects can give rise to phenomena such as metallic interfaces in multilayers of two Mott insulators, $LaVO_3$ and $LaTiO_3$, or a metal-insulator transition in the correlated metal $CaVO_3$, for which we find that both tensile strain and a reduced film thickness can lead to a strong quasiparticle renormalization [1].

[1] Beck *et al.*, Phys. Rev. B **97**, 075107 (2018).

Charge transfer at the $LaCoO_3$-$LaTiO_3$ interface

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Thin films of perovskite oxides have shown interesting properties and can be relatively easily combined, making them suitable building blocks for novel electronics. However, when perovskite thin films are combined, interface effects can strongly affect the overallproperties. Understanding these interface effects can play an important role in increasing performance of thin film based devices.
Recently, a model has been proposed by Z. Zhong and P. Hansmann[1] based on the oxygen octahedral backbone that continues across the interface between two perovskites. The oxygen 2p-bands should thereforebe aligned, creating an offset between the transition metal 3d-bands, resulting in interfacial charge transfer. The aim of this study was to gain insight in this interfacial charge transfer by investigating the non-polar $LaCoO_3$-$LaTiO_3$ interface, since the band offset between $LaTiO_3$ and $LaCoO_3$ is one of the largest[1].
Ultra-thin layers of $LaCoO_3$ and $LaTiO_3$ were grown on $LaAlO_3$-buffered $SrTiO_3$ and $LaAlO_3$ substrates by Pulsed Laser Deposition. Subsequently, X-ray Absorption Spectroscopy and photoemission techniques have been used to determine the valence of the transition metal ions. Scanning Transmission Electron Microscopy in combination with Electron Energy Loss Spectroscopy (STEM-EELS) was used to find the spatial distribution of transition metal valence.
In $LaCoO_3$, the expected Co^{3+} valence was observed. However, when $LaCoO_3$ was sandwiched between $LaTiO_3$, a strong Co^{2+} signal emerged, up to a 100% Co^{2+} signature for a 2 unit cell thick $LaCoO_3$ layer. Systematically changing the $LaCoO_3$ thickness and monitoring the Co^{2+} to Co^{3+} ratio, allowed to quantify the charge transfer to about 1.5 electron per unit cell interface. In STEM-EELS, a Co^{2+}signal was observed at the interface, in a region of about 3 unit cells. Furthermore, the charge transfer seems independent of temperature or substrate choice.
In conclusion, we've found a significant charge transfer at the interface between $LaTiO_3$ and $LaCoO_3$. Interfacial charge transfer seems a promising way to doping materials without disrupting the structure, thereby enabling novel properties.

[1] Z. Zhong and P. Hansmann, Phys. Rev. X 7, 011023 (2017)

Growth of superconducting Sr_2RuO_4 thin films

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Sr_2RuO_4 is an unconventional superconductor with potentially a spin-triplet, odd-parity superconducting ground state. There are many reports of high purity single crystals of Sr_2RuO_4 with a T_c of up to 1.5 K. Furthermore, recent studies on Sr_2RuO_4 single crystals have shown that the T_c can be further increased up to 3.5 K using uniaxial strain. To date, however, there are only three published reports of superconducting Sr_2RuO_4 thin films. This relative paucity of superconducting thin films is likely due to the extreme sensitivity of the odd-parity superconducting ground state in Sr_2RuO_4 to disorder. According to recent theoretical predictions biaxially strained epitaxial thin films with isotropic in-plane strain can potentially maintain the topologically nontrivial $p_x \pm ip_y$ superconducting ground state while simultaneously enhancing T_c by tuning the Fermi level towards a van Hove singularity. Thin films also provide a pathway for scalability, which is critical for potential practical applications of spin-triplet superconductors, such as qubits for ground-state quantum computing. Here, we outline and demonstrate a thermodynamic growth window to achieve repeatable growth of superconducting Sr_2RuO_4 with higher T_c than all prior thin films using molecular-beam epitaxy. We will also present some preliminary evidence of epitaxial strain-induced tuning of T_c.

In-situ imaging of electric field-induced ferroelastic domain motion in $SrTiO_3$

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$SrTiO_3$ displays superconductivity, incipient ferroelectricity and can host two-dimensional electron gases (2DEGs). These phenomena occur below the cubic-to-tetragonal transition, where ferroelastic twins emerge as a result of the lower symmetry and have a strong impact on all the aforementioned properties. To shed light on these issues, we exploited the magnetoelastic coupling caused by the imprinting of ferroelastic domains into magnetostrictive films on $SrTiO_3$. With this approach we could image the spatial distribution of ferroelastic twins under the action of in-situ applied electric fields and revealed the expected anisotropic dielectric behaviour of tetragonal $SrTiO_3$ [1]. Based on first-principles and Landau theory, we associate the observed anisotropy to the emergence of an antiferroelectric (AFE) lattice instability of the Ti ions that couples to polar and AFD lattice modes. The appearance of this coupling also solves the longstanding issue of the origin of the R-point infrared-active phonon which previously was generically assigned to the back-folding of the Brillouin zone in the tetragonal phase. Our study foresees the emergence of antiferroelectric instabilities in other oxide perovskites, a prediction that deserves further research in the lattice dynamics of these materials.

[1] B. Casals, Physical Review Letters, in press.

Emergent Properties of Dirac and Weyl Semimetals of Iridates

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Fusion of strong correlation and quantum topology may provide a new arena for materials physics toward emerging quantum technology. Here, we target the Ir-oxides with orthodox structures of perovskite ($AIrO_3$) and pyrochlore ($R_2Ir_2O_7$), which are both characterized by strong electron correlation and large spin-orbit coupling. In those compounds, intriguing magneto-transport properties emerge in the proximity of the Mott transition, such as unusually high electron mobility, large thermoelectric effect, large topological Hall response, and large magnetoresistance in the symmetry-protected Dirac semimetal states of $AIrO_3$ and the magnetic-order-induced multiple Weyl semimetal states of $R_2Ir_2O_7$.

Berry phase engineering at oxide interfaces

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Geometric phases in condensed matter play a central role in many intriguing phenomena such as the quantum, spin and anomalous Hall effect. In contrast to the quantum Hall effect, which is characterized by a global topological invariant and robust against perturbations, the anomalous Hall effect depends on the Berry curvature of occupied bands at the Fermi level and is therefore highly sensitive to subtle changes in the band structure. A unique platform for its manipulation is provided by transition metal oxides, owing to the delicate balance between energy scales and the possibility of creating atomically sharp interfaces, where nanometer-scale electronic and magnetic reconstructions can occur. We demonstrate how electronic transport in the ultrathin ferromagnetic oxide $SrRuO_3$ can be manipulated by imposing asymmetric boundary conditions in the form of two dissimilar interfaces. Measurements of the AHE, which probe the Berry curvature of occupied bands, reveal the presence of two spatially-separated, spin-polarized conduction channels. Using theoretical calculations we show that the Berry curvature of the spin-polarized Ru bands is modified near the $SrTiO_3$ and $SrIrO_3$ interfaces, resulting in opposite signs of the anomalous Hall conductivity. Our study demonstrates how reconstructions at oxide interfaces can be used to control spin and charge accumulation on a nanometer-scale, opening new routes towards spintronics and topological electronics.

Quantum transport in the films of a magnetic semiconductor $EuTiO_3$

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$EuTiO_3$ (ETO) is a magnetic semiconductor, in which $4f^7$ moment on Eu^{2+} site orders in G-type antiferromagnet below 5.5 K and into ferromagnet under a magnetic field above 3 T. Electron carriers are doped in Ti t_{2g} conduction band by the substitution of Eu^{2+} with La^{3+}. We previously reported that a metalorganic gas source molecular beam epitaxy (MOMBE) at very high substrate temperature materializes the high electron mobility quantum well system of La-doped $SrTiO_3$ (STO) that can host quantum Hall effect [1]. We have extended the synthesis to compressively strained $EuTiO_3$ films to observe novel Hall effect arising from magnetic monopole at the Wyle nodes created by crystal-field and Zeeman splitting of Ti $3d$ bands [2].
We now discuss the transport properties of 100 nm thick $Eu_{1-x}La_xTiO_3$ films grown on lattice-matched STO substrates by the MOMBE. Despite the magnetic moment on Eu site, which is unfavorable condition for the mobility compared with STO case, the electron mobility exceeds 3,000 $cm^2V^{-1}s^{-1}$ at 2 K, Shubnikov-de Haas (SdH) oscillations being clearly observable in high magnetic field. This quantum transport provides opportunities to discuss the detailed band structures with taking into account the Zeeman splitting and exchange coupling between Eu $4f$ and Ti $3d$ electrons. The discussion will be extended to quantum well structures of $EuTiO_3$.

[1] Y. Matsubara, K. S. Takahashi et al., Nat. Commun. 7 11631 (2016).
[2] K. S. Takahashi et al., to be published.

Ferroelectrically tunable magnetic skyrmions in ultrathin oxide heterostructures

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Magnetic skyrmion is a topologically protected whirling spin texture in nanoscale.[1] Its small size, topologically-protected stability, and solitonic characteristics together hold great promises for future spintronics applications.[2] To translate such compelling features into practical spintronic devices, a key challenge lies in achieving effective control of skyrmion properties, such as size, density, and thermodynamic stability. Here, we report the discovery of ferroelectrically tunable skyrmions in ultrathin $BaTiO_3$/$SrRuO_3$ bilayer heterostructures.[3,4] The ferroelectric proximity effect at the $BaTiO_3$/$SrRuO_3$ heterointerface can trigger a sizable Dzyaloshinskii-Moriya interaction, thus stabilizing robust high-density skyrmions. The skyrmion size in this system can be minimized down to approximately 10 nm. Moreover, by manipulating the ferroelectric polarization of the $BaTiO_3$ layer, we achieve local, switchable and nonvolatile tunability of both skyrmion density and thermodynamic stability. Such ferroelectric control of skyrmion properties heralds a novel approach to simultaneously enhance in the integratability and addressability of skyrmion-based functional devices.

[1] N. Nagaosa & Y. Tokura Nat. Nanotech. 8, 899 (2013).
[2] A. Fert, et al. Nat. Rev. Mater. 2, 17031 (2017).
[3] L. Wang et al. Nano Lett. 16, 3911 (2016).
[4] L. Wang et al. Adv. Mater. 29, 1702001 (2017).

Unraveling the Enhanced Transition Characteristics of Thermochromic VO_2 Thin Films for Energy Efficient Smart Windows

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VO_2 is an extensively studied smart thermochromic material. It exhibits a phase transition (Semiconductor-Metal Transition (SMT)) at 68 ^oC, which embeds its utility in various energy saving applications like smart windows, IR detectors, etc. Different studies have shown that the SMT characteristics can be altered with a change in defect concentration. In the present work, we have tried to understand the influence of defects on the SMT. Here we report the single step synthesis of VO_2 thin films on glass substrates by chemical vapor deposition (CVD) at 520 ^oC. The as-deposited films were annealed at 200 ^oC. The as-deposited films and annealed films are all polycrystalline with the monoclinic crystal structure (($P2_1/c$)). XPS analysis of the as-deposited films revealed the presence of oxygen vacancies. With annealing, oxygen might diffuse through the boundaries. This was verified from both XPS and R-T analyses. We inferred that annealing of VO_2 thin films deposited on glass substrates, enhances the transition characteristics. An increase in resistance by an order of magnitude in the annealed films was observed. From this study, we understand that the oxygen vacancies modify the phase transition in VO_2 thin films on glass substrates and its electrical properties.

All inorganic electrochemical transistor with correlated oxides for low power and thermally stable artificial synapses

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Synapse, a combination of memory and information processing units, is the ultimate goal to emulate for electronic devices. They outperform a conventional von-Neumann architecture in terms of information processing speed and energy efficiency. Recent studies mimicked synaptic functions and minimized energy per synaptic event by using a phase change memory (100 fJ for 100 nm^2 device area)[1] and an organic electrochemical transistor (10 pJ for 1000 μm^2 device area)[2], but the energy consumption is still greater than that of the biological synapse (10 fJ). In addition, the organic electronic devices have been showed unreliable property at high temperature which is not appropriate for practical applications. Correlated oxides exhibit high thermal stability due to the inorganic nature as well as a strong electron correlation in narrow d-band that result in extremely sensitive electrical properties to their electronic configuration. They exhibit electrical phase transition by external stimuli, so-called a metal-to-insulator transition, which are not only consuming less energy but also faster, making them suitable for use in high-speed and low-power neuromorphic devices. Recently, hydrogen is reversibly injected into $SmNiO_3$, which gives rise to the non-volatile resistivity change of 10^8 orders of magnitude.[3]

In this study, we have demonstrated an inorganic electrochemical transistor using a $NdNiO_3$ thin film as a channel layer and a porous silica film as a proton exchange membrane. As an electric field is applied to a gate electrode, a positively charged protons migrate into or out of the $NdNiO_3$ channel layer. As a result, the channel conductance switches due to a change in the proton doping concentration in the $NdNiO_3$ layer. The devices showed nonvolatile and distinct multilevel conductance switching, and synaptic functions. In addition, it has achieved low gate pulse amplitude (50 mV), energy efficiency (1.8 pJ for 4000 μm^2 device area), and thermally stable operation up to 200 ^oC. It will guide the development of thermally stable neuromorphic device that can catch up with the energy efficiency of biological synapses.

[1] Kim, I. S. et al. High performance PRAM cell scalable to sub-20nm technology with below 4F2 cell size, extendable to DRAM applications. 2010 Symposium on VLSI Technology 203-204 (IEEE, 2010).

[2] Van de Burgt, Y. et al. A non-volatile organic electrochemical device as a low-voltage artificial synapse for neuromorphic computing. Nat. Mater. 16, 414-418 (2017).

[3] Shi, J., Zhou, Y. & Ramanathan, S. Colossal resistance switching and band gap modulation in a perovskite nickelate by electron doping. Nat. Commun. 5, 4860 (2014).

Characteristics of Laser-Induced Terahertz Emissions from Gallium Oxide Surfaces

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Laser terahertz (THz) emission microscopy/spectroscopy (LTEM/LTES) is a non-contact evaluation technique based on THz emission spectroscopy and imaging that can visualize intensity of pulsed terahertz radiations from the materials and devices excited by femtosecond laser pulses. LTEM/LTES enables the visualization of the dynamic responses of photoexcited carriers in a sample [1-4]. We have applied this technique to characterize various materials and devices for far and demonstrated the potential of LTEM/LTES as a novel inspection technique.

In this study, we measured gallium oxide (β-Ga_2O_3) that is recently attracting significant attention as a candidate for next generation power electronics by using LTEM/LTES [5]. The characteristics of THz emissions from Ga_2O_3 surfaces were systematically investigated and the results showed clear dependences of THz waveforms on carrier concentrations, surface orientations and plane angles of polarization of excitation laser pulses. Moreover, we compared the LTEM and photoluminescence (PL) images and found that the distribution of THz emission intensity was much different from that of PL intensity. From these results, we will discuss the THz wave generation mechanism in the Ga_2O_3 surfaces, and potential of LTEM/LTES as an evaluation method of Ga_2O_3.

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[1] D. S. Rana et al., Advanced Materials, Vol. 21, 2881 (2009)
[2] Y. Sakai et al., Scientific Reports 5, 13860 (2015)
[3] Y. Sakai et al., APL Photonics 2, 041304 (2017)
[4] F. R. Bagsican et al., Scientific Reports, Vol. 7, 1774 (2017)
[5] M. Higashiwaki et al., Appl. Phys. Lett., Vol.100, 013504 (2012)

Selective gas sensing using WO_3 nanoparticles and zeolites hybrid structure for human cutaneous gas sensors

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Improvement of gas sensors using WO_3 nanoparticles is acquired by integrating a zeolite layer into gas sensors. It could be fundamental base of hybrid sensors using multiple gas sensors with different zeolites represent improved selectivity.

Metal oxide semiconductor nanoparticle based gas sensors are widely used for health care gas sensors, detecting the respiratory and cutaneous gases from human body and it makes disease screening possible. Especially, WO_3 gas sensors shows remarkable sensing qualities comparable to SnO_2 with high signals to ammonia, hydrogen sulfide, and acetone. It is the reason why WO_3 is the only two metal oxide semiconductor based gas sensors in commercial application. [1-3] Despite of its common applications, there is a problem of gas selectivity on WO_3 gas sensors that not only target gases but also many kinds of gases are reacted with WO_3 nanoparticles. Considering that porous zeolites show the various gas absorption characteristics by different pore sizes. [4] By applying porous zeolites have different pore sizes on the gas sensors, it is expected to get high selectivity by adsorbing targeted gases onto zeolites. In addition that, combination with many kinds of gas sensors which have different gas sensitivity shows much better performance of sensors by signal analysis of each sensor.

In this study, two different types of zeolites onto WO_3 gas sensors are fabricated and get the better selectivity for low pressure of acetone gas from human skin surface. At the end of this experiments, fabrication of WO_3 nanoparticle based gas sensors are insensitive to the other gases except acetone is expected and it would be suitable health-care application for personal diet progress examination.

Semiconductor (WO_3 nanoparticle) gas sensors covered with zeolitic films (FAU or LTA) have been developed and used forgas phase sensing of different species (acetone, ethanol and ammonia) at different gas concentrations. The dynamic responsesobtained with these sensors were compared with the response of a reference sensor without a zeolitic layer. The results clearlyindicate that a suitable zeolite layer strongly reduces, and in some cases suppresses, the response of the sensor to large molecules,thereby increasing the sensor selectivity to the small molecules, while the reference sensor could not discriminate between thesemolecules. Additionally, using the characteristic of gas adsorption of zeolites, the sensor could be exposed to higher gas concentration compared with the reference sensor and this phenomena is occurred in case that the molecule size is similar with pore size of the zeolite. This clearly shows the potential of zeolite-based sensors to achieve a higher selectivity/sensitivity in gas sensing applications. And these sensors, although they are composed of same semiconductor material, the target gas could be intentionally and differently controlled by using various pore size of zeolites. Through hybrid gas sensors, the correlation between the gas adsorption rate in the zeolitic layer and the mass of zeolite is studied.

[1] A. Staerz et al., Sens. and Actuators B, 237(2016), 54
[2] L. Valentini et al., Thin Solid Films, 436 (2003), 95
[3] T. Toyooka et al, J. Breath Res., 036005(2013)
[4] Y. Yamada et al, Anal. Chem., 7588(2015), 87

Micro-mechanical resonators powered by oxides' solid state phase transitions: a VO_2-based micro-engine

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VO2 undergoes a solid state phase transition (SSPT) at about 65°C, which results in a drop of its electrical resistivity by more than three orders of magnitude and a change of lattice symmetry from low temperature monoclinic phase to high temperature tetragonal one. Remarkably, its phase transition is intrinsically fast (ps) and it occurs in a sharp temperature window of 5- 10 °C, with hysteresis between the heating and cooling branches. The strong coupling between electronic and lattice transition makes this material an ideal candidate as functional element in new micro/nano-electro-mechanical systems.

We take advantage of this SSPT to perform high-frequency mechanical actuation of micro and nano-electro-mechanical devices[1]. The actuating scheme relies on the non-linear behavior of VO2 that triggers a spontaneous periodic phase transition between its insulating/monoclinic and metallic/tetragonal phases. This periodic electrical and structural instability is used to excite the flexural modes of a micromechanical resonator. This actuation mechanism has unique points of strength if compared with other approaches, since it allows the simple and direct transduction of a DC voltage bias into a mechanical excitation in the MHz range, while typical methods to achieve resonant electrical actuation rely on active electronics to generate AC excitation signals.

This approach to resonant actuation will enable the design of simple and autonomous micro/nano electromechanical devices with integrated DC power sources, like solar cells or small batteries. Our scheme could impact in a variety of fields of applications, like robotics, environmental monitoring or biomedical sensors (see also: www.vo2actuators.spin.cnr.it).

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[1] N. Manca, L. Pellegrino, T. Kanki, W. J. Venstra, G. Mattoni, Y. Higuchi, H. Tanaka, A. D. Caviglia, and D. Marré, Adv. Mater. 29, 1701618 (2017).

Magnetoresistance behaviors of conducting filaments in resistive-switching NiO with different resistance states

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Resistive switching (RS) effect in various materials has attracted much attention due to its interesting physics and potentials for applications. NiO is an important system and its RS effect has been generally explained by the formation/rupture of Ni related conducting filaments. These filaments are very unique since they are formed by electroforming process, so it is interesting to explore their magnetoresistance (MR) behaviors, which can also shed light on the unsolved issues, such as the nature of the filaments and their evolution in the RS process, etc., and is also important for multifunctional devices. We have studied the RS effect of NiO thin films grown on Pt/Ti/SiO2/Si substrates by using various techniques. Direct observation of Ni filaments and different magnetizations for the low resistance state and high resistance state in NiO were realized and a multifilamentary picture for the process of filament rupture during the RESET process was revealed. We also studied the MR behaviors in NiO RS films with different resistance states. Rich and interesting MR behaviors have been observed for the unique Ni conducting filaments formed in the NiO RS samples, including the normal AMR with a positive AMR ratio, the anomalous AMR with a negative AMR ratio, superposition of the normal AMR and the anomalous AMR, and even sign change of the AMR ratio with decreasing temperature. We also observed the TMR behavior in some samples with the high resistance state which is a new breakthrough, indicating a nano-magnetic tunnel junction can be realized in the Ni filament just by the RESET process. Through the experimental results and first-principles calculation, we provide an in-depth understanding of the Ni conducting filament in the NiO RS samples, such as the size of Ni filaments related to the RS effect, microscopic evolution process of the filaments in the RS process, and the location of the filaments rupture region. Our work provides a new avenue for the exploration of the conducting filaments in resistive switching materials and shed light on the nature of the filaments and their evolution in the RS process, which are significant for understanding the mechanism of RS effect and multifunctional devices.

Growth and characterization of epitaxial La-doped $BaSnO_3$ thin films grown by pulsed laser deposition

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Transparent conducting oxides (TCOs) have attracted attention due to their unique properties and potential applications in various modern optoelectronic and electronic devices[1,2]. Recently, the transparent perovskite La-doped $BaSnO_3$ has gained considerable attention as a novel TCO due to its room temperature high-mobility, which is higher than most TCOs and other perovskite oxides[3,4].
Compared to bulk single crystals, La-doped $BaSnO_3$ epitaxial thin films show reduced mobility[5,6]. However, in order to fully explore the potential for device applications and novel physics phenomena in La-doped $BaSnO_3$, there is a need to grow high-quality thin films that exhibit improved transport properties over a wide temperature range. Current research efforts concentrate on understanding the origin of the limited electron mobility and its improvement beyond the present mobility limits in epitaxial thin films[2−6].
We will report developments on the fabrication and characterization of epitaxial thin films of La-doped $BaSnO_3$ by pulsed laser deposition on different single crystal substrates. Transport properties of grown films with various La-doping will be discussed. The electronic band structure of the thin films, probed by angle-resolved photoemission spectroscopy, will also be presented.

[1] H. Ohta, K. Nomura, H. Hiramatsu, K. Ueda, T. Kamiya, M. Hirano, and H. Hosono, Solid State Electron. 47, 2261 (2003).
[2] W.-J. Lee, H. J. Kim, J. Kang, D. H. Jang, T. H. Kim, J. H. Lee, and K. H. Kim, Annu. Rev. Mater. Res. 47, 391 (2017) and references therein.
[3] H. J. Kim, U. Kim, T. H. Kim, J. Kim, H. M. Kim, B-G. Jeon, W-J. Lee, H. S. Mun, K. T. Hong, J. Yu, K. Char, and K. H. Kim, Phys. Rev. B 86, 165205 (2012).
[4] H. J. Kim, U. Kim, H. M. Kim, T. H. Kim, H. S. Mun, B-G. Jeon, K. T. Hong, W-J. Lee, C. Ju, K. H. Kim, and K. Char, Appl. Phys. Express. 5, 061102 (2012).
[5] C. Park, U. Kim, C. J. Ju, J. S. Park, Y. M. Kim, and K. Char, Appl. Phys. Lett. 105, 203503 (2014).
[6] P. V. Wadekar, J. Alaria, M. O'Sullivan, N. L. Flack, T. D. Manning, L. J. Phillips, K. Durose, O. Lozano, S. Lucas, J. B. Claridge, and M. J. Rosseinsky, Appl. Phys. Lett. 105, 052104 (2014).

Monolithic integration of patterned $BaTiO_3$ thin films on Ge wafers

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Titanates exhibit electronic properties highly desirable for field effect transistors such as very high permittivity and ferroelectricity. However, the difficulty of chemically etching titanates hinders their commercial use in device manufacturing. Here, we report the selective area in finestra growth of highly crystalline $BaTiO_3$ within photolithographically defined openings of a sacrificial SiO_2 layer on a Ge (001) wafer by molecular beam epitaxy. After the $BaTiO_3$ deposition, the sacrificial SiO_2 can be etched away, revealing isolated nanoscale gate stacks circumventing the need to etch the titanate thin film [1]. Reflection high-energy electron diffraction in conjunction with scanning electron microscopy is carried out to confirm the crystallinity of the samples. X-ray diffraction is performed to determine the out-of-plane lattice constant and crystal quality of the $BaTiO_3$ film. Electrical measurements are performed on electrically isolated $Pt/BaTiO_3/SrTiO_3/Ge$ capacitor devices.

[1] P. Ponath, A. B. Posadas, M. Schmidt, A.-M. Kelleher, M. White, D. O'Connell, P. Hurley, R. Duffy and A. A. Demkov, *Monolithic integration of patterned $BaTiO_3$ thin films on Ge wafers*, J. Vac. Sci. and Technol. B **36** (2018).

The Fermi energy in oxides: Assessing and understanding the limits using XPS

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The Fermi energy in semiconductors can often be freely controlled across the whole energy gap by doping. This is not the case in oxides, where different mechanisms exist, which can limit the range of the Fermi energy. These limits can be caused by i) dopants having deep rather than shallow charge transition levels, ii) by self-compensation where the Fermi energy dependence of the formation energy leads to spontaneous formation of compensating defects, iii) the change of the oxidation state of either the cations or the oxygen. The latter is particularly relevant for compounds with transition metal or rare earth cations. This presentation will demonstrate that the limits of the Fermi energy can be assessed using X-ray photoelectron spectroscopy (XPS). The variation of the Fermi energy can thereby be achieved either by deposition of thin films on different substrates, by deposition of differently doped films, by different surface treatments including oxygen and vacuum annealing, oxygen plasma treatments and water adsorption, or by formation of interfaces with low and high work function metal oxides. The presentation will give an overview on the experimental approach and its limitations and demonstrate the observation of the different limitation mechanisms. The effects will be illustrated using extensive data sets for various oxides, including differently doped $SrTiO_3$, $BaTiO_3$, $Pb(Zr,Ti)O_3$, $(La,Sr)FeO_3$, $(La,Sr)MnO_3$, $BiFeO_3$, $LaAlO_3$, $BiVO_4$, CeO_2, Fe_2O_3, Co_3O_4, Bi_2O_3, ZnO, In_2O_3, SnO_2, NiO, Cu_2O, MgO, Al_2O_3 and SiO_2.

InteractiveXRDFit: a new tool to simulate and fit X-ray diffractograms of oxide thin films and heterostructures

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InteractiveXRDFit is a Matlab program that calculates the X-ray diffracted intensity for heterostructures. Other fitting programs are already available and efficient, but may lack some flexibility with some of the parameters that this program allows modifying. Here the user can choose the substrate and the different materials composing an heterostructure among a long list of compounds (mainly perovskite oxides), choose between (001) or (111) substrate orientation, and play with the different structural parameters (unit-cell size and number of layers). It is possible to build a superlattice composed of up to three different materials, and add a top and/or bottom layer (to simulate electrodes, spacers or capping layers). Each layer can have a different c-axis (either constant or varying as a function of depth within a layer). The simulation is quick and allows the user to compare it directly to the measurements, so as to rapidly determine the crystalline parameters of the sample.

Epitaxial growth of high quality $DyBa_2Cu_3O_{7-\delta}$ using Atomic Layer by Layer Molecular Beam Epitaxy

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Artificial heterostructures provide a novel approach to systematically investigate the phase diagram of high-temperature superconducting cuprates. Recently it was demonstrated that the entire phase range from antiferromagnetic insulating, spin-density wave, superconducting and charge-density wave state can be reproduced in a single $YBa_2Cu_3O_{7-\delta}$ layer stack as a function of distance from the interface to $La_{2/3}Ca_{1/3}MnO_3$ in a superlattice [1]. In this study, an important role has been assigned to the long-range charge transfer across the interfaces, and therefore structural sharpness and cation intermixing are crucial parameters. So far, such complex multilayers have been mostly grown by pulsed-laser deposition (PLD). Oxide Molecular Beam Epitaxy (MBE), with ozone as the oxidant, allows forming atomically sharp oxide interfaces and layer specific charge doping through a chosen layer stacking sequence. [2,3] As a first step towards the goal of growing multilayer, we succeeded to grow high-quality, epitaxial $DyBa_2Cu_3O_{7-\delta}$ thin films with superconducting transition temperatures of 88 K. In contrast to previous MBE growths, the elements were deposited consecutively layer-by-layer without co-deposition. The stoichiometry and the formation of the 123-cuprate phase were controlled by using in-situ reflection high-energy electron diffraction and monitoring the periodic oscillations of intensities of different diffraction spots. Scanning-transition electron microscopy confirms the atomically sharp substrate-film interface and the absence of stacking defaults, previously observe in PLD grown heterostructures.

[1] A. Frano et al., *Long-range charge density wave proximity effect at cuprate-manganate interfaces*, Nat. Mater. **15**, 2016.
[2] F. Baiutti et al., *High-temperature superconductivity in space-charge regions of lanthanum cuprate induced by two-dimensional doping*, Nat. Commun. **6**, 2015.
[3] F. Wrobel et al., *Comparative study of $LaNiO_3$ /$LaAlO_3$ heterostructures grown by pulsed laser deposition and oxide molecular beam epitaxy*, Appl. Phys. Lett. **110**, 2017.

Epitaxially stabilized phase and oxygen vacancy-ordering in cobaltite (double-)perovskite thin films

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Atomic structure is one of the most crucial parameters determining the physical properties in perovskite oxides, including electron transport, magnetism, and ion transport. Among the broad range of available perovskites, cobaltates take a distinct position as a result of the low valence state desired by the cobalt B-site cation: Compensating the 2+/3+ mixed valence state of cobalt, perovskite structures with large oxygen substochiometry ($\delta \approx 0.5$) can be generated. As a result, cobaltates can stabilize ordered oxygen-vacancy structures bearing the potential to exploit structural ordering phenomena as an additional degree of freedom for the design physical and chemical properties. Epitaxy uniquely allows to stabilize such degrees of freedom by exploiting growth kinetics and epitaxial strain.

Besides the intrinsic interest of our oxide electronics community in synthesis control and electronic transport, these compounds moreover bridge our field to the field of electrochemistry, where (ordered) cobaltate double perovskites are being widely explored as catalysts for water splitting applications, paving ground for a novel field of research where expertise in complex oxide synthesis is highly desired. In this study, we show that atomic ordering can be stabilized in (100) $(Pr_{0.5}Ba_{0.5})CoO_{3-\delta}$ (PBCO) thin films, characterized by coherent ordering of oxygen vacancies in every second $CoO_{2-\delta}$ atomic plane, forming a meta-stable Brownmillerite-like atomic structure. [1] The formation of this ordered phase occurs during synthesis and can be observed in-situ using reflection high energy electron diffraction (RHEED). Ordered phase formation is fully controlled by growth temperature, whereas vacancy-ordering is stabilized when exceeding a growth temperature of 900°C and providing sufficiently oxidizing conditions. In contrast, growth at low oxygen pressure promotes CoO-secondary phase precipitation. Based on X-ray diffraction, we observe that structural ordering occurs fully coherent and in parallel to the (100) thin film-substrate interface. Using atomic scale imaging (HRSTEM) and analysis (SEDX), we show that oxygen-vacancy ordering is the prevalent ordering phenomenon in PBCO, while the mixed A-site cations, Ba and Pr, remain fully disordered.

We discuss electronic transport properties of ordered and disordered thin films, exhibiting hopping-type conduction that shows significant strain-dependence and vanishes upon reduction of the PBCO thin films. The thin films are moreover applied as model catalysts for electrochemical water splitting, complementing their oxide electronic application. As we show, rather than atomic ordering, it is the electrical conductivity of the cobaltate layer that promotes catalytic performance as well as enhanced current densities and reaction rates accessible for water splitting. [2] The observed effect illustrates the importance of catalyst surface chemistry, while physical design rules for catalysts based on bulk structural arguments fail.

[1] F. Gunkel et al., ACS Catalysis 7, 7029-7037 (2017)

[2] M. Weber et al., Chem. Mater. (submitted)

Deposition and Nanofabrication of All Perovskite $YBa_2Cu_3O_{7-y}$/Ferromagnetic/ $YBa_2Cu_3O_{7-y}$ Josephson Junctions

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The competition between spin-singlet superconductivity and magnetic ordering in superconductor/ferromagnet (S/F) heterostructures gives rise to a variety of unusual physical phenomena. One of them is the generation of a long-range odd-frequency spin-triplet component of the superconducting order parameter in the F-layers [1]. This effect should be most pronounced and unambiguous in case of fully spin-polarized ferromagnets, which do not support the existence of spin-singlet Cooper pairs, such as the colossal magnetoresistance manganites [2]. In this line we present our recent results on the fabrication and characterization of all-perovskite SFS junctions made of high-temperature cuprate superconductor $YBa_2Cu_3O_{7-y}$. Different ferromagnetic oxides have been utilized as the ferromagnetic spacer: the ruthenate $SrRuO_3$ and the manganites $La_{2/3}Ca_{1/3}MnO_3$ and $La_{2/3}Sr_{1/3}MnO_3$, both individually and combined in Spin Valve (SV) arrangements. Our heterostructures have been deposited on $La_{0.3}Sr_{0.7}Al_{0.65}Ta_{0.35}O_3$ (LSAT) substrates via Pulsed Laser Deposition (PLD). In order to probe the perpendicular transport through these S/F/S structures, as we successfully did on a former collaboration [3], nanoscale junctions have been made by photolithography, Reactive Ion Etching and Focused Ion Beam milling. These structures will be soon electrically characterized in order to study the influence of the magnetic profile of the junction in the modulation of the Josephson current.

[1] F. S. Bergeret, A. F. Volkov, and K. B. Efetov, Rev. Mod. Phys. **77**, 1321 (2005).
[2] S. Jin, M. McCormack, T. H. Tiefel and R. Ramesh, Journal of Applied Physics **76**, 6929 (1994).
[3] T. Golod, A. Rydh, V. M. Krasnov, I. Marozau, M. A. Uribe-Laverde, D. K. Satapathy, Th. Wagner, and C. Bernhard, Phys. Rev. B **87**, 134520 (2013).

$LaVO_3$ Thin Films under Epitaxial Strain

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The interplay between spin, charge, orbital and lattice degrees of freedom is extremely strong and at the origin of numerous phenomena in complex oxides [1]. The bulk $3d^2$ AVO_3 (A being a rare-earth) showcases an interesting phase diagram where the low temperature orbital and spin orderings are strongly dependent upon the A cation size [2]. The $GdFeO_3$-type distortions remove the t_{2g} orbital degeneracy to generate a Mott state. Above the Jahn-Teller transition temperature, orbitals fluctuate between the quasi non-degenerated t_{2g} energy levels [3].
For $LaVO_3$, below the transition temperature (140 K), a spontaneous G-type orbital ordering concomitant with a C-type spin ordering arises along the long orthorhombic axis.
We have explored the effect of biaxial strain in epitaxial thin films of $LaVO_3$ [4]. X-ray diffraction reveals that the layers accommodate the strain imposed by the substrate assuming different patterns of octahedral tilts and rotations. These structural changes have been predicted by *ab-initio* theory. We used temperature dependent X-ray diffraction, muon spectroscopy and optical conductivity to investigate the strain effect on the orbital and magnetic transitions.

[1] D. I. Khomskii, Transition metal compounds (Cambridge University Press, 2014).
[2] Y. Ren *et al.*, Nature (London) **396**, 441 (1998); Phys. Rev. B **67**, 014107 (2003).
[3] M. De Raychaudhury, E. Pavarini, and O. Andersen, Phys. Rev. Lett. **99**, 126402 (2007).
[4] H. Meley *et a.*, APL Materials **6**, 046102 (2018).

Stoichiometry and epitaxial strain control of electrocatalytic activity in Ruthenate thin films

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Oxygen evolution reaction (OER) occurring at the anode of water splitting electrolyzer plays an essential role for the utilization the hydrogen energy. Particularly, the lower efficiency compared to hydrogen evolution reaction led to intensive studies on the materials with high OER activity. Perovskite transition metal oxides are drawing remarkable attentions as promising catalysts, especially with its ability to facilitate the electronic structure for the fundamental understanding of the OER mechanism. Indeed, electronic structures of perovskite oxides, highly relevant for the electrocatalytic activity can be largely manipulated through elemental vacancy engineering and epitaxial strain within a single material system. In this study, we fabricated coherently strained high-quality $CaRuO_3$ (CRO) epitaxial thin films on various substrates using pulsed laser epitaxy (PLE). To manipulate the electronic structure, we tuned both the stoichiometry and the epitaxial strain of the thin film. We used optical spectroscopy for the identification of the evolution of the electronic structure near the Fermi energy. The optical transitions among different electronic bands are systematically controlled via the film stoichiometry as well as epitaxial strain, providing the evolution of the fundamental electronic structure. Cyclic-voltammetry was employed to examine the OER activity, which showed large variation despite the small change within the CRO thin film system. The result shows strong correlation between the Ru-O hybridization and the OER activity. In particular, the strong hybridization within the material hampers the fluent transport of charges for the electrocatalytic activity. The understanding of OER activity based on fundamental electronic structure of transition metal oxides will provide an important guideline for identifying adequate activity descriptor for the electrocatalytic performances.

Effect of symmetry mismatch on the heteroepitaxial growth of T-Nb_2O_5 on $SrTiO_3$

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Nb_2O_5 is an interesting compound for resistive switching applications. However, its functional properties are rarely investigated due to the lack of available single-crystals. To overcome this issue high-quality epitaxial films have to be fabricated on foreign substrates because native substrates are not available. In this context, not only the lattice parameter mismatch, but also the symmetry difference between film and substrate material have to be considered.

In this paper, we investigate the effect of symmetry mismatch on the epitaxy of T-Nb_2O_5 on the prototype perovskite substrate $SrTiO_3$. An important aspect of the difference in symmetry between these two materials is the connection between the oxygen octahedra. In $SrTiO_3$ the TiO_6 octahedra are connected by their corners, whereas in T-Nb_2O_5 the oxygen octahedra (NbO_6) are connected by their corners and edges. It is found that the difference in lattice parameter and symmetry results in the formation of domains that have the b-axis of T-Nb_2O_5 aligned along the $SrTiO_3$ <001> in-plane directions. Hence, the number of domain orientations is four and two for the growth on (100)- and (110)-oriented substrates, respectively. However, the out-of-plane growth direction remains the same for both substrates orientations. Analysis of the interface structure by transmission electron microscopy reveals that the first atomic layers of Nb_2O_5 on (110)-oriented $SrTiO_3$ adopt a structure that is different from the bulk and rather resembles an ABO_3 perovskite structure, but with a significant amount of A-site cation vacancies. This implies that for the first monolayers the oxygen octahedra in this Nb_2O_5 structure are solely connected by their corners similar to the octahedra network in the perovskite substrate. The transition to the T-Nb_2O_5 structure with the bulk like symmetry and oxygen octahedra connection occurs via a few nanometer thin disordered interface region. We believe that this transition is accompanied by a local variation of the valency of Nb ions allowing for a change of local coordination, i.e. type of connection of oxygen octahedra. These results thus show that a meta-stable phase can be stabilized by means of epitaxial growth on a symmetry mismatched substrate and also help to advance our understanding of the growth of symmetry mismatch materials.

Epitaxial growth of La_2NiMnO_6 thin films on STO by RF Sputtering

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La_2NiMnO_6 (LNMO) is an insulating ferromagnet and as such, could be a good candidate for magnetically active insulating barrier in spin filters. In this work epitaxial thin films have been prepared on (001) oriented $SrTiO_3$ substrates by RF magnetron sputtering using different growth conditions. The effects of the oxygen pressure (PO2) and growth temperatures on the microstructure, magnetic and transport properties of the films have been investigated. 20-50 nm thick films grow fully strained showing insulating behavior irrespective to the growth conditions used. However, microstructure (Ni/Mn ratio) and magnetic properties strongly depend on oxygen pressure conditions. High oxygen pressures promotes the growth of stoichiometric films, with Ni:Mn ≈ 1 , but degraded magnetic properties with surface segregates. In contrast, films grown at low oxygen pressure exhibit Ni/Mn ratios below 1:1 indicating a deviation from the ideal double perovskite structure and with some Mn excess, which induces an increased B-site cationic disorder and the increase of Mn^{3+} content. Nevertheless, off-stoichiometry films are fully strained and exhibit high crystallinity with flat and clean surfaces, insulating behavior with optimal magnetic properties and T_c around 270 K.

[1] Nyrissa S.Rogado, Jun Li, Arthur W. Sleight, and Mas A. Subramanian. Adv. Mater, 17, 2225-2227 (2005).
[2] Min Zhu,Yong Lin, Edward W. C. Lo, Qiong Wang, Zhengjie Zhao, and Wenhui Xie, Appl. Phys. Lett. 100, 062406 (2012).
[3] M. Kitamura, I. Ohkubo, M. Kubota, Y. Matsumoto, H. Koinuma, and M. Oshima, Appl. Phys. Lett. 94, 132506

Domain matching epitaxy and modified interfacial layer in $BaBiO_3$ thin films on $SrTiO_3$

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The perovskite $BaBiO_3$ (BBO) is a versatile oxide parent material which displays superconductivity upon p-doping, while n-doping has been predicted to establish a wide-bandgap topological insulator phase [1].

We report on the mechanism that allows for epitaxial deposition of high-quality crystalline BBO thin films on $SrTiO_3$ (STO) substrates despite a significant lattice mismatch of as large as 12%. By transmission electron microscopy it is revealed that the growth takes place through domain matching epitaxy, resulting in domains with alternating lateral sizes of 8 and 9 BBO unit cells. A structurally modified interfacial layer of 1.7 nm thickness serves as a nucleation layer for the BBO films, since it gradually relieves the strain by decoupling the film lattice from the substrate [2].

Raman spectroscopy on BBO films of various thicknesses indicates the persistence of the bulk lattice symmetry down to a film thickness of 3 nm. Below this thickness, the Raman signal vanishes, confirming the structural differences of the bismuthate lattice close to the interface to STO. Our in situ XPS characterization furthermore evidences that the first deposited film layers are Bi deficient, resulting in modifications of the electronic structure of the thinnest films.

The BBO growth mechanism identified here may be prototypical for prospective thin film deposition of other perovskites with large lattice constants.

[1] Yan et al., Nat. Phys. 9, 709 (2013)

[2] Zapf et al., Appl. Phys. Lett. 112, 141601 (2018)

Oxygen diffusion in epitaxial oxide heterostructures with $SrMoO_3$ thin films

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Transition metal perovskite oxide SrMoO3 with Mo^{4+} $4d^2$ electronic configuration reveals a room-temperature resistivity of 5.1 $\mu\Omega$cm in single-crystal form and, therefore, is considered as a prominent conducting electrode material for oxide microelectronic devices [1]. $SrMoO_3$ thin films with resistivity values down to 20 $\mu\Omega$cm at room temperature have been reported [2,3]. However, stabilization of the unfavorable Mo^{4+} valence state in $SrMoO_3$ films requires reductive growth conditions incompatible with highly-oxidative environment, which is necessary to achieve desirable stoichiometry and electron structure of many other functional oxide materials (e.g. tunable dielectric $Ba_xSr_{1-x}TiO_3$). In order to enable $SrMoO_3$ functionality, we have investigated oxygen diffusion in epitaxial oxide heterostructures comprised of $SrMoO_3$ films in combination with thin functional perovskite oxides $SrTiO_3$, $BaTiO_3$, $Ba_{0.5}Sr_{0.5}TiO_3$, and $SrZrO_3$. The valence states of the transition metal cations as Ti, Zr, and Mo were investigated in these materials at different oxidation conditions using X-ray photoelectron spectroscopy. Among the investigated materials, the lowest oxygen diffusion has been observed in $Ba_{0.5}Sr_{0.5}TiO_3$. A $Ba_{0.5}Sr_{0.5}TiO_3$ film with a thickness of only 5 unit cells preserves the Mo^{4+} oxidation state in the $SrMoO_3$ underlayer at the used oxygen partial pressure of 3 mTorr and temperature of 630 °C. Thus, $SrMoO_3$ thin films covered with atomically thin $Ba_{0.5}Sr_{0.5}TiO_3$ remain conducting in oxygen environment and can be integrated into all-oxide thin-film heterostructures together with other functional materials.

[1] I. Nagai *et al.*, *Highest conductivity oxide $SrMoO_3$ grown by a floating-zone method under ultralow oxygen partial pressure*, Appl. Phys. Lett. **87**, 024105 (2005)

[2] L. Alff *et al.*, *The role of cationic and anionic point defects in pulsed laser deposition of perovskites*, J. Phys. D: Appl. Phys. **47** 034012 (2014)

[3] A. Radetinac *et al.*, *Highly conducting $SrMoO_3$ thin films for microwave applications*, Appl. Phys. Lett. **105**, 114108 (2014)

Study of structural properties of ultrathin SrO films deposited on $SrTiO_3$

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The electronic reconstruction taking place at some selected functional oxides interfaces is known to have important effects inducing modifications of the electrical properties of the parent compounds. The ability to control the termination of substrates is crucial in order to obtain high-quality interfaces. Here we investigate structural evolution of SrO thin films with different thickness deposited on top of $SrTiO_3$(STO) substrate terminated by TiO_2. Films were deposited by means of pulsed laser deposition. AFM and XRD study shows expansion of c axis of SrO, indicates to compressive in-plane strain at SrO/STO interface. Moreover, different morphology caused by self-organization of SrO depending on substrate surface coverage and post-annealing was observed.

Substrate Preparation and High-Temperature Stoichiometry Control of Oxide Surfaces

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To study the high-temperature epitaxy on oxide surfaces, we have built a substrate heater system based on a 1 kW, 9.27 μm wavelength CO_2 industrial cutting/welding laser. Light at this wavelength is efficiently absorbed by oxides, while being reflected to a large extent by metals, allowing the use of metallic sample holders up to the melting point of sapphire. The setup includes beam shaping optics to create a top-hat beam profile, zoom lenses to adjust the beam size, and a selectively transparent Bragg mirror to enable on-axis access of a long-wavelength pyrometer for temperature control.
We find that oxide substrates such as $SrTiO_3$ (001) may be prepared for epitaxy by an in-situ high-temperature annealing procedure instead of the traditional ex-situ HF etch and oven anneal. The temperature profile consists of a rapid ramp to 1300 °C followed by a 200 s waiting time and the return to the growth temperature of 840 °C. The oxygen background pressure is 7.5 Pa (0.075 mbar) during the entire sequence. During the high-temperature step, the surface forms atomically smooth terraces limited in size by the intrinsic miscut of the crystal surface. Homoepitaxy, as well as $LaAlO_3/SrTiO_3$ interfaces and magnetic layers grown on such substrates show similar or better characteristics than nominally identical structures grown on chemically prepared substrates. This procedure works, with appropriately adjusted temperatures and oxygen pressures, also for $LaAlO_3$ and $NdGaO_3$, two other widely used substrate materials. It may therefore be applicable to a wide range of oxide substrates.
During the anneal cycle, we often observe surface reconstructions in RHEED on the up side of the temperature ramp that differ from the final one on the down ramp at the same temperature. By abruptly turning off the heating laser at any temperature, we are able to quench the substrates with temperature drops as large as 400 K during the first second. AFM 'Snapshots' from substrates quenched during heating from 1200 °C and at the end of the 200 s annealing plateau at 1300 °C show different patterns. Whereas large terraces with straight ML high steps are present in both, the phase image shows wide stripes of different surface reconstruction along the step edges at 1200 °C that have vanished at 1300 °C. These results are consistent with a model of additional SrO remaining at the surface, modifying the kinetics and causing different phase-separated surface reconstructions even at temperatures well above typical growth temperatures. Only the desorption of excess SrO at 1300 °C finally allows the surface to reach a uniformly reconstructed state. The model agrees with calculations predicting the desorption of 1 ML of SrO in 100 s at 1300 °C.[1] The non-volatility of such non-stoichiometric adatom populations at substrate temperatures beyond the usual layer-by-layer growth regime opens up new possibilities to control and modify the growth of oxide heterostructures.

[1] Bharat Jalan, Pouya Moetakef, and Susanne Stemmer, Applied Physics Letters 95, 032906 (2009); doi: 10.1063/1.3184767

The fine phase control of pyrochlore iridates epitaxial films using sequential pulsed annealing epitaxy

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Due to the large spin orbit coupling (SOC) and comparably large electron-correlations, pyrochlore iridates, $R_2Ir_2O_7$ (with R=rare earth element), will be the fertile playground for correlated topological phases [1]. The bulk pyrochlore iridates are predicted to have Weyl semimetal state which possesses topologically protected bulk and surface states at the Fermi surface [2]. In addition, recent theoretical studies revealed the emergence of a new topological phase of which are hidden in the bulk and manifest only in the thin films [3-5]. In spite of these exotic phenomena, not many experimental studies are done on these compounds due to extreme difficulty of their synthesis. The multiple oxide phase of iridium presents a key difficulty in the growth of such thin film samples.
Here, we report a high quality $Nd_2Ir_2O_7$ thin film grown on YSZ substrates by pulsed laser deposition, using a special in-situ growth technique called sequential pulsed annealing epitaxy. Layer-by-layer growth was monitored by both RHEED and in-situ spectroscopical ellipsometry. The high quality of the film is supported by the scanning transmission electon microscopy and X-ray diffraction. Our results indicate that reducing the formation of Ir and IrO_3 during the growth process are the crucial processes that determine the quality of the thin films. We expect that these findings pave the way towards the growth of high-quality pyrochlore iridates films, and more generally of oxide thin films with volatile constituents.

[1] W. Witczak-Krempa et al., Annu. Rev. Condens. Matter Phys. (2014).
[2] X. Wan et al., Phys. Rev. B (2011).
[3] B.-J. Yang et al., Phys. Rev. Lett. (2014).
[4] K. Hwang and Y. B. Kim, Sci. Rep. (2016).
[5] P. Laurell and G. A. Fiete, Phys. Rev. Lett. (2017).

Transparent thin film transistors of polycrystalline SnO_{2-x} and epitaxial SnO_{2-x}

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We report on transparent high mobility thin film field effect transistors (TFT) based on polycrystalline SnO2-x and epitaxial SnO2-x. TFTs based on polycrystalline SnO2-x of top and bottom gate geometries exhibited high mobility values of 145.79 cm2/Vs and 160 cm2/Vs, respectively. The TFTs also showed high Ion/Ioff ratios and the subthreshold swing values were 0.29 V/dec and 0.71 V/dec, respectively. However, our polycrystalline SnO2-x devices showed non-ideal behavior in their output and transfer characteristics; a large hysteresis was observed both in their output and transfer characteristics. The most probable origin for these non-ideal behaviors is the barrier formation across grain boundaries of polycrystalline SnO2 [1].

In order to confirm this, we used epitaxial SnO2-x grown on r-plane sapphire substrates as a channel layer, and compared performances with those of polycrystalline SnO2-x based TFT. We will discuss the effect of epitaxial SnO2-x on the disappearance of the hysteretic behavior.

[1] M. Batzill and U. Diebold, Prog. Surf. Sci. 79, 47 (2005)

Tuning Interfacial Ferromagnetism via Crystallographic Symmetry Mismatch

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Creating and tuning ferromagnetism at the interfaces between two non-ferromagnetic materials is of fundamental and technological interest. At the interface of antiferromagnetic $CaMnO_3$ (CMO) perovskite layer a fractional charge transfer can stabilize magnetic ground state which is highly sensitive to local structural distortions. Therefore, inducing subtle structural modifications at the $CaMnO_3$ interface can lead to large changes in magnetization. Here two scenarios will be discussed:

• **Superlattices of crystallographically similar perovskites: $CaMnO_3$ - $CaRuO_3$.**
Interfacial ferromagnetism can be modified by making an interface between two crystallographically similar perovskites: $CaMnO_3$ and $CaRuO_3$ (CRO) but with different orientations thus inducing a symmetry mismatch at the interface via octahedral rotations.[1] CMO/CRO superlattices with even and odd number of "pseudocubic" CMO unit cells exhibit very different interfacial saturation magnetization: 1.0 μ_B/Mn and 0.5 μ_B/Mn, respectively. This difference is difficult to explain within the existing theoretical framework. Using x-ray diffraction, it was found that growing even or odd number of CMO unit cells in a CRO/CMO superlattice results in different octahedral rotation patterns. Here, it will be shown how these distortions affect magnetization in even/even, even/odd, odd/even, and odd/odd superlattices.

• **Superlattices of crystallographically different perovskites: $CaMnO_3$ - $LaNiO_3$.**
The interface between two crystallographically different perovskites: the orthorhombic CMO perovskite exhibiting the $a^-a^-c^+$ octahedral rotations and the rhombohedral $LaNiO_3$ (LNO) exhibiting $a^-a^-a^-$ rotations shows very different magnetization behavior.[2] In LNO/CMO superlattices the octahedral connectivity across the LNO/CMO interface can be controlled by changing the LNO and CMO layer thicknesses as well as their relative ratio and this way effectively alter the balance between ferromagnetic and antiferromagnetic interactions in the interfacial CMO layer. It was found that in LNO/CMO superlattices, the interfacial ferromagnetism can be modulated by a factor of three. The origin of the interfacial ferromagnetic variation is directly related to changes in Mn-O-Ni and Mn-O-Mn bond angles and bond lengths.

The results demonstrate a path for creating and controlling the magnetic state via octahedral connectivity at the interfaces between two non-ferromagnetic materials with similar as well as distinct crystallographic symmetries.

[1] A.J. Grutter, et al., Nano Lett. **16**, 5647 (2016).
[2] C.L. Flint, et al., Phys. Rev. B **96**, 144438 (2017).

Robust 2D Skyrmions in ultra-thin $SrRuO_3$ film

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The magnetic skyrmions have fast evolved from a novelty, as a realization of topologically protected object with particle-like spin texture, toward to device application as a magnetic storage [1, 2]. Moreover, we can see a big progress with the synthesis of new material showing room-temperature skyrmions in a variety of magnetic material and artificial heterostructures [3], where the geometry of the structure induces interfacial Dzyaloshinskii-Moriya Interactions (DMI) conducive to the skyrmion formation.
Here, we would like to present our findings of 2D skyrmion formation in a simple thin-film structure consisting with a few perovskite unit cell of $SrRuO_3$ grown on top of $SrTiO_3$ substrate. Moreover, the 2D skyrmion is very much strong/robust without any capping layer for artificially boosting the effective DMI [3, 4]. The Topological Hall Effect (THE) as a fingerprint of the skyrmion show robust and stability of the topological particle (skyrmion), considering from the high critical field $\mu_0 H \sim 1.57$ Tesla (T) at low temperature. Surprisingly, THE survived as the field is tilted by as high as 85 degree at 10 K, or up to the in-plane external magnetic field strength of ~ 6.5 Tesla. We propose that the robustness is derived by the strong magnetic anisotropy, which is strongly related with magnetic domain/domain wall formation in the ultra-thin $SrRuO_3$ film. We believe the deep understanding of this robust 2D skyrmions can help to design new type of future magnetic storage application.

[1] N. Nagaosa and Y. Tokura, Nat. Nanotech. **8**, 899 (2013).
[2] W. Jiang, G. Chen, K. Liu, J. Zang, S. G. E. Velthuis, A. Hoffmann, Phys. Rep. **704**, 1 (2017).
[3] J. Matsuno *et al.*, Sci. Adv. **2**, e1600304 (2016).
[4] C. Moreau-Luchaire *et al.*, Nat. Nanotech. **11**, 444 (2016)

Defect-induced exchange bias in a single $SrRuO_3$ layer

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Exchange bias stems from the interaction between different magnetic phases and therefore it generally occurs in magnetic multilayers. Here we present a large exchange bias in a single $SrRuO_3$ layer induced by helium ion irradiation. When the fluence increases, the induced defects not only suppress the magnetization and the Curie temperature, but also drive a metal-insulator transition at a low temperature. In particular, a large exchange bias field up to $\sim 0.36\,\mathrm{T}$ can be created by the irradiation. This large exchange bias is related to the coexistence of different magnetic and structural phases that are introduced by embedded defects. Our work demonstrates that spintronic properties in complex oxides can be created and enhanced by applying ion irradiation.

Mechanical strain engineering of magnetism in $PrVO_3$ thin films

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The transition- metal oxides with ABO_3 type structure show a strong spin - orbital and lattice coupling, implying that the lattice distortion plays an important role in tuning the electronic and magnetic properties of ABO_3 perovskites. Previous study shows that the chemical strain engineering in PVO films by monitoring the concentration of oxygen vacancies can tune the Neel temperature (T_N) of PVO films in range of 30 K [1]. We present an experimental study of magnetic response to the residual strain in $PrVO_3$ thin films grown on a variety of single crystal substrates by pulsed laser deposition (PLD), producing different strain states in $PrVO_3$ thin films from -4.7% (compressive) to 0.5% (tensile). $PrVO_3$in bulk, being a strong anti-ferromagnet shows Neel temperature 130 K [2]. Our study reveals that the lattice distortion via misfit strain pave the way towards tuning the anti-ferromagnetic ordering temperature in $PrVO_3$ thin films, resulting in a non-trivial evolution of the Neel temperature (T_N) with substrate pseudo-cubic lattice parameter. We demonstrate that the strain produced via mechanical strain engineering, tune T_N of PVO films in the range of 90 K. We also show that $PrVO_3$ thin films show low temperature ferromagnetic behavior along with the insulating properties irrespective of the substrate.

[1] O. Copie et. al. Adv. Mater. 1604112, (2017)
[2] Sage M H et. al. Phys. Rev. B 76 195102 (2007)

What does and does not lie behind emergent thickness-dependent ferromagnetism in $LaMnO_3$ films

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Above a critical thickness of six unit cells, high quality, polar $LaMnO_3$ films grown epitaxially on non-polar $SrTiO_3$-(001) substrates using PLD switch to a ferromagnetic state, as shown beautifully by scanning SQUID microscopy [1]. Using samples from the same laboratory as [1], we use hard X-ray photoemission (HAXPES), soft X-ray resonant photoemission and soft X-ray absorption (XAS) in both linear (XLD) and magnetic circular dichroism (XMCD) modes to uncover what is and is not driving this remarkable phenomenon.

HAXPES picks up no polar build-up in the LMO at any thickness, and strong divalent Mn signals are observed in both XAS and HAXPES for films as thin as n=2 unit cels. The extreme sensitivity of XMCD uncovers magnetically polarisable Mn 3d spins even for n=2, but with a remnant moment of only 0.1 μ_B. The HAXPES and XAS analysis shows the average manganese valency to smoothly increase from majority divalent (60% 2+) for n=2 to minority divalent (25% 2+) for n=7 and excludes tetravalent Mn throughout. The XMCD sum rules clearly pick up the emergent ferromagnetism for n>6 as a six-fold[ten-fold] jump in the remnant Mn magnetic moment between n=2 and 7 [10] unit cells. XLD analysis shows that the Mn favours an in-plane orbital ordering at all thicknesses. The X-ray spectroscopy data are matched perfectly by cross- sectional TEM-EELS, showing a zone of divalent Mn at the LMO—STO interface.

The overall picture may not be exotic, but it is clear. Below the critical thickness, the LMO is too electron-rich and too close to both the substrate and surface to sustain ferromagnetism. Above n=6, the average valency matches that for the FM phases seen in hole-doped $La_{1-x}Sr_xMnO_3$, and the ferromagnetism wins out above the influence of the well-known interfacial dead layers. Given the clear exclusion of self-doping, oxygen vacancies may prove to be the cheapest source of electron-doping of the manganese.

[1] Wang et al., Science 349, 6249 (2015)

$SrRuO_3$ as a Model System for Quantum Dots of Correlated Materials

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For several decades quantum dots or artificial atoms have been attracting attention as zero-dimensional electron systems due to their remarkable electronic properties [1]. In conventional quantum dots made of semiconductors or metals, correlation effects, if existing, arise mainly from the quantum confinement induced for example by lateral patterns, superlattices, electric fields or magnetic impurities leading to Kondo-type behavior [2,3].
Here we propose and present artificial atoms fabricated from materials with inherently correlated electron systems [4]. Size-quantization effects generated by confinement of such materials into quantum dots may cause significant modifications of the already existing correlated electron system and lead to properties that are not present in other materials.
As a material for fabrication of artificial atoms we use $SrRuO_3$ [5] grown on $SrTiO_3$ (100). The quantum dots are grown by pulsed laser deposition and patterned by electron beam lithography with the spatial resolution down to 20 nm.
We will show that the quantum dots have enhanced magnetic properties as compared to the epitaxial films. This enhancement we find to be caused by a modified strain distribution in the $SrRuO_3$.

[1] 1. R. C. Ashoori, Electrons in artificial atoms, Nature 379 (1996) 413-419
[2] 2. T. Chakraborty, Physics of the artificial atoms: quantum dots in a magnetic field, Comments Cond. Mat. Phys. 16 (1992) 35-68
[3] 3. M. Ternes, A. J. Heinrich, W.-D. Schneider, Spectroscopic manifestations of the Kondo effect on single adatoms, J. Phys.: Condens. Matter 21 (2008) 053001
[4] 4. J. Mannhart, H. Boschker, T. Kopp, R. Valenti, Artificial atoms based on correlated materials, Rep. Prog. Phys. 79 (2016) 084508
[5] 5. G. Koster, L. Klein, W. Siemons, G. Rijnders, J. S. Dodge, C.-B. Eom, D. H. A. Blank, M. R. Beasley, Structure, physical properties, and applications of SrRuO3 thin films, Rev. Mod. Phys. 84 (2012) 253-298

Ultrafast control of the Morin phase transition in the magnetic oxide $DyFeO_3$ by phonon pumping

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Ultrafast magnetism has rapidly developed over the past years into a large research field, since control over magnetization on the picosecond time scale can have an enormous impact on today's data storage and technology. Essential to this field is the use of ultrashort, high-energy laser pulses (<100 fs) to both bring the magnetic materials out of equilibrium and study the resulting dynamics on the femtosecond scale in time-resolved pump-probe experiments. Transition metal oxides, which often exhibit strongly correlated electron physics, have emerged to offer a very interesting playground, in which the spin, charge and lattice degrees of freedom are tightly coupled and are very susceptible to ultrafast optical stimuli in both the optical and mid-IR frequency range.

In this research we focus on the ultrafast photo-induced emergence of a net magnetization across the first-order Morin phase transition in $DyFeO_3$, using ultrashort mid-IR pulses (200 fs, 6-18 μm) resonant with a phonon band around the Fe-O stretching phonon mode. This transition takes the material from a compensated collinear to a noncollinear antiferromagnetic state. We study the transition in an all-optical time-resolved pump-probe experiment and explore the underlying driving mechanism. We shows that the resonantly perturbed lattice gives rise to a change of the magnetic anisotropy of the material, following a non-thermodynamic pathway that couples, out of equilibrium, structural and magnetic instabilities. In addition, the presence of a 'coexistence region', between the true antiferromagnetic, low-temperature phase and the weakly ferromagnetic, high-temperature phase in the H-T phase diagram of the material turns out to be essential. In this region, the two phases have similar energy scales and the system becomes highly susceptible to perturbations. We explore and utilise this coexistence to induce and study the ultrafast changes in magnetization.

Polarised Neutron Reflectivity Study of Magnetic Oxides Thin Films using HANARO Reflectometers

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Polarised neutron reflectometry (PNR) has been offering unique opportunities for investigating magnetic surfaces and interfaces in both condensed and soft matter materials. The high penetration depth of neutron, the variation of scattering length with isotopic nuclei, and the sensitivity on magnetic spin enable to study the morphology of magnetic oxide thin films and the magnetic anisotropy in heterostructures. HANARO (High-flux Advanced Neutron Application Reactor) neutron facility in Korea has been expanding polarized neutron reflectivity capabilities since the completion of the cold neutron guide in 2008. For magnetic oxides, neutron polariser/guides, 4K cryocooler, and electromagnet have been upgraded. Study of exchange coupling and magnetic anisotropy in magnetic layered heterostructures was conducted using polarised neutron reflectivity measurement. In this presentation, the HANARO reflectometers and current research will be presented.

Ferrimagnetic Skyrmion in a Charge-transfer Superlattice

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Exploring exotic interface magnetism due to charge transfer in perovskites has profound application in future development of spintronic memory. In this study, $CaMnO_3/CaIrO_3$ superlattice is found to possess interface ferrimagnetism by charge transfer, perpendicular magnetic anisotropy up to room temperature, as well as Topological Hall Effect (THE) indicating the presence of magnetic Skyrmion. Emergence of Skyrmions in such symmetric, antiferromagnet/paramagnet oxide superlattice is very novel, and its stabilization is further explained by an "interfacial roughness model". The abrupt suppression of THE by large current allows extraction of Skyrmion threshold current density of 10^8 $A/m^2$and current dependent Skyrmion drift velocity. This discovery opens an innovative route in stabilizing the Skyrmion phase in oxide hetero-structure.

[1] Matsuno J, Ogawa N, Yasuda K, Kagawa F, Koshibae W, Nagaosa N, et al. Interfacedriven topological Hall effect in SrRuO3-SrIrO3 bilayer. Sci. Adv. 2016, 2(7): e1600304.
[2] Nichols J, Gao X, Lee S, Meyer TL, Freeland JW, Lauter V, et al. Emerging magnetism and anomalous Hall effect in iridate-manganite heterostructures. Nat. Commun. 2016, 7: 12721.
[3] Schulz T, Ritz R, Bauer A, Halder M, Wagner M, Franz C, et al. Emergent electrodynamics of skyrmions in a chiral magnet. Nat. Phys. 2012, 8: 301.

Tailoring magnetic oxide quantum wells

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The fabrication of artificial heterostructures has enabled interface and size control of complex oxide materials, for which unique phenomena with no bulk analogues have been demonstrated. Going beyond oxide surfaces and interfaces, the next simplest heterostructure is a quantum well (QW). Quantum size effects make it possible to tailor the effective band gap of the oxide material and control its optical, magnetic and electronic properties in emerging applications-in terms of quality that were thought to be unique to semiconductors.

The basic idea of quantum confinement-using potential gradients caused by band offsets or band bending-applies to complex oxides just as to conventional semiconductors, but the physics is much richer. For example, using oxides with intrinsic magnetic order allows to combine spin-related phenomena with optoelectronic applications.

In this context, europium monoxide (EuO) shows remarkable properties: It is a strong ferromagnet with a Curie temperature of TC= 69K and a bulk magnetic moment of 7muB. EuO undergoes a large magnetization-driven insulator- to-metal transition below TC , displays large magnetooptical effects and can generate up to 100% spin-polarized electron currents if employed as a magnetic tunnel barrier. Interestingly, even fundamental optical properties, such as the nature of the band gap-direct or indirect-remain a subject of debate and often have to rely on the works published many decades ago before high-quality EuO thin films became available.

Our advances in the growth of EuO now make it possible to study magnetic and optoelectronic properties down to the few atomic layer limit [1]. Quantum wells are created from ultrathin single-crystalline EuO layers to study the evolution of the optical band gap down to the single nanometer regime. The excellent single-crystalline layer and interface quality of the YSZ/EuO/MgO heterostructures grown by MBE were confirmed by RHEED, XRD and XRR [1,2].

Using infrared transmission spectroscopy, we have demonstrated that that the EuO band gap is indirect - independent of quantum well thickness - and increases from 1.19 eV for bulk-like (d=32 nm) to 1.4 eV in the ultrathin films (d=1.1 nm). We find a blue shift of the EuO absorption edge of up to 0.2 eV and a reduced effective mass of the electron-hole pair of mu=mo The observed band-gap widening is a clear sign of a quantum confinement effect, which can be used to control and modify the band gap in EuO-based all-oxide heterostructures and provides aroute for engineering the band gap in complex magnetic oxides for emerging spin- and optoelectronic applications [2].

[1] G. Prinz, T. Gerber, A. Lorke, and M. Müller, Appl. Phys. Lett. 109, 202401 (2016)

[2] G. Prinz, M. Ney, P. Lömker, A. Lorke, and M. Müller (in preparation)

Non-collinear magnetism and "living-dead" layer in rare earth titanate thin films

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Among transition-metal perovskites, rare-earth orthorhombic titanates $RTiO_3$, (R=La...Lu or Y) emerge as a particularly interesting family of Mott-Hubbard insulators [1]. The most stable valence state of rare-earths (except for Eu and Ce) is 3+, which imposes a 3+ valence state to the Ti, that is thus $3d^1$ with a spin 1/2. A salient feature of $RTiO_3$ compounds is the phase transition from ferrimagnetic to antiferromagnetic (G-type) order when going from small (Lu...Gd) to large rare-earths (La...Sm) [1,2]. This insulating-ferrimagnetic behaviour is exceptional among simple perovskites and offers perspectives for engineering novel magnetic states at oxide interfaces [3,4].

The growth of high quality thin films of rare-earth titanates is very challenging due to the relatively poor stability of the Ti^{3+} valence state. So far, literature on ferrimagnetic compounds is very scarce, aside from some reports on $GdTiO_3$ films by oxide molecular beam epitaxy [5] and a few on $YTiO_3$ films grown by pulsed laser deposition [6, 7]. Here, we will report on the epitaxial growth of high-quality, single-phase films of different ferromagnetic titanates, with special emphasis on $DyTiO_3$. We will show that while thick films (>40 nm) have bulk-like magnetic properties, with high remanence and a Curie temperature near 60 K, in thinner films a paramagnetic component develops at the expense of the ferromagnetic one. We will analyze and discuss this effect in terms of deviations from the 3+ Ti valence state at the film surface [8].

Finally, we will show the first detailed XAS and XMCD investigation on this family of compound. By combining several detection modes during Ti $L_{2,3}$ XAS measurements, we could gain further insight on the depth dependence of the Ti valence and magnetism. Interestingly, the XMCD on Ti $L_{2,3}$ edge present a non-zero integral on certain member of the $RTiO_3$ family, which, according to the sum rules, implies a non-zero orbital moment.

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[1] J. B. Goodenough et al., J. Phys.: Condens. Matter 17, 7395-7406 (2005)
[2] M. Mochizuki et al., PRL 91, 167203 (2003)
[3] M. N. Grisolia et al., Nature Physics 12, 484-492 (2016)
[4] G. Conti et al., Journal of Applied Physics 113, 143704 (2013)
[5] P. Moetakef et al., J. Vac. Sci. Technol. A 31, 041503 (2013)
[6] Y. Cao et al., APL 107, 112401 (2015)
[7] S. C. Chae et al., APL 89, 182512 (2006)
[8] R. Aeschlimann et al., Adv. Mat. In print (2018)

Complex Oxide Heterostructures for Spin Electronics

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The generation and manipulation of pure spin currents from magnetization dynamics in ferromagnetic layers is an ongoing research field that has gathered much attention in the past twenty years. When the spins of a ferromagnetic layer, which is in contact with a non-magnetic one, start to precess coherently, a pure spin current is injected into the non-magnetic film in a process known as spin pumping (SP). The physics underlying this effect are still not well understood, but empirical evidence suggests that the spin-orbit coupling of the non-magnetic film is crucial. Spin-orbit coupling is also responsible for the inverse spin hall effect (ISHE), i.e. the conversion of a pure spin current into a charge current, which opens the possibility to measure it electrically. In this work, we carry out spin pumping and ISHE measurements in ferromagnetic/non-magnetic thin film structures composed of Permalloy/Pt as well as La0.67Sr0.33MnO3 (LSMO)/Pt. Both SP and ISHE measurements will be performed, by using a coplanar waveguide ferromagnetic resonance spectrometer, as a function of external magnetic field and temperature. SP and ISHE, and the contrary process, i.e. spin Hall effect (SHE), are of much recent interest because of their very promising prospects for the development of spintronic devices.

Strain-induced high-temperature perovskite ferromagnetic insulator

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Ferromagnetic insulators are required for many new magnetic devices, such as dissipationless quantum-spintronic devices, magnetic tunneling junctions, etc. Ferromagnetic insulators with a high Curie temperature and a high-symmetry structure are critical integration with common single-crystalline oxide films or substrates. So far, the commonly used ferromagnetic insulators mostly possess low-symmetry structures associated with a poor growth quality and widespread properties. The few known high-symmetry materials either have extremely low Curie temperatures ($\leq$16 K), or require chemical doping of an otherwise antiferromagnetic matrix. Here we present compelling evidence that the LaCoO3 single-crystalline thin film under tensile strain is a rare undoped perovskite ferromagnetic insulator with a remarkably high TC of up to 90 K. Both experiments and first-principles calculations demonstrate tensile-strain-induced ferromagnetism which does not exist in bulk LaCoO3. The ferromagnetism is strongest within a nearly stoichiometric structure, disappearing when the Co2+ defect concentration reaches about 10%. Significant impact of the research includes demonstration of a strain-induced high-temperature ferromagnetic insulator, successful elevation of the transition over the liquid-nitrogen temperature, and high potential for integration into large-area device fabrication processes.

[1] Dechao Meng, Hongli Guo, Zhangzhang Cui, Chao Ma, Jin Zhao, Jiangbo Lu, Hui Xu, Zhicheng Wang, Xiang Hu, Zhengping Fu, Ranran Peng, Jinghua Guo, Xiaofang Zhai, Gail J. Brown, Randy Knize, and Yalin Lu, PNAS 115 (12) 2873-2877 (2018)

Magnetic tunnel junctions based on ferroelectric $Hf_{0.5}Zr_{0.5}O_2$ tunnel barriers

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In ferroelectric tunnel junctions, devices composed of two electrodes sandwiching a ferroelectric tunnel barrier, the transmission can be strongly modulated by the direction of the ferroelectric polarization, inducing giant tunnel electroresistance (TER) with ON/OFF ratios reaching 10^4, and opening a new path for high-density ferroelectric memories [1]. Ferroelectric tunnel barriers can also be integrated between two magnetic electrodes, creating artificial multiferroic tunnel junctions (MFTJ), displaying both TER and TMR (tunnel magnetoresistance) with high potential for multilevel memories [2].
In the last past years, intensive research has been conducted on hafnia-based thin films due to their unexpected ferroelectricity, usually appearing when size down scaled to around 10 nm or below, and to their CMOS compatibility [3]. Very recently, the fabrication of a ferroelectric tunnel junction based on $Hf_{0.5}Zr_{0.5}O_2$(HZO) ultrathin film has been reported and a TER ratio of 20 was demonstrated, attesting the potential of HZO as ferroelectric tunnel barrier [4]. However, up to now, HZO has not been integrated yet between magnetic electrodes to investigate TMR effect and thus create multiferroic tunnel junctions.
Recently, (111)-oriented HZO films have been epitaxially grown on (001)-$La_{0.7}Sr_{0.3}MnO_3$(bottom electrode)/SrTiO3substrates, showing large ferroelectric polarization values up to 34 $\mu C/cm^2$ without the need forwake-upcycling [5]. Structural characterization reveals a rhombohedral phase, different from the commonly reported polar orthorhombic phase, allowing to propose a compelling model for the formation of the FE phase in HZO films[5].In this work, ultra-thin 2-5 nm-thick (111)-oriented HZO films have been epitaxially grown on (001)-$La_{0.7}Sr_{0.3}MnO_3/SrTiO_3$, with top electrode $La_{0.7}Sr_{0.3}MnO_3/(La_{0.7}Sr_{0.3})(Mn_{0.93}Ru_{0.07})O_3$. MTJs have been fabricated by several steps of patterning (including lithography, etching and deposition) with junction sizes of 5x5, 8x8 and 10x10 μm^2. First magneto-transport measurements have revealed a tunneling transport through HZO barrier and TMR values of around 15% at low temperature. Higher TMR values are expected by improving the antiparallel magnetic alignment between bottom and top magnetizations. With that purpose, Co top electrodes are actually under investigation for next HZO-based magnetic tunnel junctions. In addition, TER effect is being measured by Piezoelectric Force Microscopy, to study the potential of HZO tunnel barrier in MFTJs.

[1] V. Garcia and M. Bibes, Nature Communications 5, 4289 (2014). Ferroelectric tunnel junctions for information storage and processing
[2] E.Y. Tsymbal, et al.,MRS Bulletin 37, 138 (2012). Ferroelectric and multiferroic tunnel junctions
[3] M. H. Park, et al. Adv. Mater. 27, 1811-1831 (2015). Ferroelectricity and Antiferroelectricity of Doped Thin HfO2 -Based Films.
[4] F. Ambriz-Vargas, et al., Appl. Phys. Lett. 110, 093106 (2017). Tunneling electroresistance effect in a Pt/Hf0.5Zr0.5O2/Pt structure.
[5] Y. Wei, P. Nukala, M. Salverda, S. Matzen, H-J. Zhao, J. Momand, A, S. Everhardt, G. R. Blake, P. Lecoeur, B. J. Kooi, J. Íñiguez, B. Dkhil, B. Noheda, A rhombohedral ferroelectric phase in epitaxially-strained Hf0.5Zr0.5O2 thin films, arXiv:1801.09 (submitted)

Anomalous negative electroresistance and giant resistance modulation in epitaxial manganite/piezoelectric heterostructures

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The electrical control of the conductance state through phase transition and/or resistivity switching in heterostructures of strongly correlated oxides is at the core of a large research activity both for fundamental and applied interest. In an electromechanical device made of a manganite/piezoelectric heterostructure, we observe an anomalous negative electroresistance effect and a significant tuning of the metal-to-insulator transition temperature when an electric field is applied. Supported by finite element simulations, we identify the electric field applied along the conducting bridge as the plausible origin: stretching the underlying piezoelectric substrate, it gives rise to a lattice distortion of the manganite overlayer through epitaxial strain. Large modulations of the resistance are also observed by applying static dc voltages across the thickness of the piezoelectric substrate. These results indicate that the emergent electronic phase separation in the manganites can be selectively manipulated when interfacing with a piezoelectric material, which offers great opportunities in designing novel oxide-based electromechanical devices.

Orbital ordering of the mobile and localizedelectrons at oxygen-deficient $LaAlO_3/SrTiO_3$ interfaces.

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Interfacing different transition-metal oxides gives another route in functionalizing their rich interplay of electron, spin, orbital and lattice degrees of freedom for novel electronic and spintronic devices. Electronic and magnetic properties of $SrTiO_3$ based interfaces hosting a mobile two-dimensional electron system (2DES) are strongly influenced by oxygen vacancies which form a dichotomic electron system where strongly correlated localized electrons in the in-gap states (IGSs) coexist with non-correlated delocalized 2DES. Here, we use resonant soft-X-ray photoelectron spectroscopy to prove the e_g character of IGS as opposed to t_{2g} character of the 2DES in the paradigm $LaAlO_3/SrTiO_3$ interface as well as separate the d_{xy} and d_{xz}/d_{xz} orbital contributions based on a novel insight into the resonant photoexcitation process in terms of orbital and momentum selectivity. Supported by self-consistent DFT+DMFT calculations, this experiment identifies local orbital reconstruction that goes beyond the conventional e_g vs t_{2g} band ordering. A hallmark of oxygen-deficient $LaAlO_3/SrTiO_3$ is a significant hybridization of the e_g and t_{2g} orbitals. Our findings constitute a fundamental basis for new routes to understanding the interfacial magnetism and superconductivity of oxide interfaces through "defect engineering" with oxygen vacancies.

[1] F. Lechermann et al., Physical Review B 90 (8), 85125 (2014).
[2] C. Cancellieri et al., Nature Communications 7, 10386 (2016).

Interfacial octahedral coupling and dimensionality controlled electronic transitions in $NdNiO_3/SrTiO_3$ superlattices

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Rare-earth nickelates exhibiting sharp metal-insulator transitions (MITs) have attracted great interests because of the diverse emergent states arising at the heterointerfaces as well as the potential device applications. Here we studied the electronic transitions in $NdNiO_3/SrTiO_3$ superlattices by atomically controlling the layer thickness of $NdNiO_3$. The interfacial octahedral coupling resulted in a tetragonal structure with quenched in-plane octahedral tilting for all the superlattices. As a result, the superlattice with 8 uc $NdNiO_3$ layer showed a much reduced MIT temperature (T_{MI}=126 K) together with a dramatically suppressed insulating state below T_{MI} as compared to the $NdNiO_3$ single film. However, for a thinner $NdNiO_3$ layer of 6 uc, the dimension effect induced bandwidth reduction dominated over the interfacial octahedral coupling, leading to an increased T_{MI}=163 K. With further reducing the $NdNiO_3$ layer to 2 uc, a semiconducting behavior with 2D variable range hopping (VRH) conduction was observed. Also, the temperature dependent resistivity curve showed a kink around 65 K, which was a hint for the paramagnetic-antiferromagnetic transition. The decoupled MIT and magnetic transitions in the ultrathin superlattice indicate that dimensionality control can be a powerful tool to manipulate the multiple ordering states in correlated oxides.

[1] Middey S. et al., Physics of ultrathin films and heterostructures of rare-earth nickelates. Annu. Rev. Mater. Res. 46, 305-334 (2016).

Exploring the phase diagram of $Nd_{1-x}La_xNiO_3$ thin films

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Mixing together $LaNiO_3$ and $NdNiO_3$ into a solid solution thin film produces a rich phase diagram with a metal-insulator transition, a magnetictransition and two structural transitions. Characterisation of the individual phases as a function of the composition, x, is done primarily by electronic transport, x-ray diffraction and Raman spectroscopy.
The various transitions will be mapped out across composition and temperature, shedding light on the physics governing the famous nickelate phase diagram.

Phase transition induced micromechanical actuation in VO_2 coated cantilever

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Structural phase transition assisted micromechanical actuation ofVO_2 coated silicon microcantilever is presented. 300nm polycrystalline VO_2 film was deposited over silicon surface at 520°C using chemical vapor deposition technique. The as-deposited films were imaged using scanning electron microscope which indicate the formation of continuous granular film with an average crystallite size ranging from 200-250nm. The formation of M1 monoclinic phase of the as-deposited VO_2 film was confirmed by XRD studies and further verified by temperature variable Raman spectroscopy. The heated VO_2 film exhibits semiconductor-to-metal transition (SMT) at 74°C which produces change in electrical resistance almost three orders in magnitude. Consequently, theVO_2 film undergoes structural phase transition from monoclinic phase $(011)_{M1}$at room temperature to tetragonal phase $(110)_R$. This generates a compressive stress within the VO_2 film resulting in large, reversible cantilever deflection which was measured with non-contact 3D optical profilometer. This method of static deflection measurement doesn't require vacuum conditions or expensive equipment such as TEM or SEM. Also, the issues of laser spot alignment over small cantilever surface can be overcome. Upon heating, VO_2 coated silicon cantilever produced large reversible tip deflection of 14 μm at 50°C. Several heating and cooling cycles indicate steep change in cantilever tip deflection with negligible hysteresis. In addition, the effect of thermal stress induced cantilever deflection was estimated to be as small as 6.4% and hence can be ignored. These results were found to be repeatable within controlled experimental conditions.

Mott Variable-Range Hopping Transport in Sr_2IrO_4 Epitaxial Thin Films

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TheJeff= 1/2 Mott insulator Sr2IrO4has attracted attention due to its novel electronic states originating from coexisting strong spin-orbit interaction and electron correlation. Themagnetic, electronic, and structural similarity of this system to undoped cuprates such as La2CuO4, has led to theoretical predictions of new superconducting states [1,2]. The d-wave gap symmetry that has been recently observed with surface-electron doping [3,4] has reinforced this expectation. However, no superconducting transport property has been discovered in this compound up to this point. Moreover, it is puzzling that electron-doped Sr2IrO4 thin films such as (La,Sr)2IrO4 [5] display robust insulating behavior, while electron-doped Sr2IrO4 bulk crystals show metallic transport [6].

In this presentation, we report that Sr2IrO4 thin films under lattice strain and chemical pressure show robust 3D Mott variable-range hopping (VRH) transport, r (T) = r0 exp (TM /T)1/4, where the characteristic temperature (TM) is related to the disorder of the system. One can expect that disorder would be increased by increasing strain, hence enhancing TM. However, our experimental data show the opposite behavior: Samples under larger strain (for both compressive and tensile) have smaller TM than samples with minimal strain. We note that TM is inversely proportional to the density of states at the Fermi energy (N(EF)) [7]. The smaller TM values of the strained samples mean that lattice strain results in doping of carriers in this system. For tensile strain, we speculate that a small number of oxygen vacancies are introduced in the samples. For compressive strain, cation off-stoichiometry, e.g. interstitial Sr ions, are presumably responsible for the increased N(EF). The magneto-transport data of our samples show negative and positive magnetoresistance at high and low temperatures, respectively, which means that the transport mechanism is governed by a disorder induced localization and electron-electron correlations. Ca and Ba doped Sr2IrO4 thin films also show consistent TM behavior as compared with the compressive and tensile strained thin films, respectively. We will discuss this robust Mott VRH transport in Sr2IrO4 thin films in comparison with other thin film Mott insulators such as La2CuO4 and LaMnO3.

[1] F. Wang and T. Senthil, Phys. Rev. Lett. 106, 136402 (2011).
[2] H. Watanabe, et al, Phys. Rev. Lett. 110, 027002 (2013).
[3] Y. K. Kim, et al, Science 345, 187 (2014).
[4] Y. K. Kim, et al, Nat. Phys. 12, 37 (2016).
[5] J. Ravichandran, et al, J. Phy.: Condens. Matter 28, 505304 (2016)
[6] M. Ge, et al, Phys. Rev B 84, 100402 (2011)
[7] N. F. Mott, J. Non-Cryst. Solids 1, 1 (1968).

Bad-metalicity and microstructure in rare-earth nickelates

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Rare-earth nicklates ($RENiO_3$) are known to display sharp metal-insulator transitions (MIT) [1], which hold great promise as memristive devices for neuromorphic computing or resistive switching applications. The transition temperature (T_{MI}) is determined by the Ni-O-Ni angular configuration (octhahedral tilts), which can be tuned by varying the radius of RE ion, applying hydrostatic pressure or, in the case of epitaxial films, by altering the lattice mismatch between film and substrate [2]. Despite the vast amount of recent work on these materials[3], the origin of their metal-insulator transition, their bad-metal behaviour [4,5] and thickness tunability are still not fully understood, mainly due to difficulties in the control on the sample homogeneity and microstructure[6]. In this work, we investigate the correlation between the transport properties and the microstructure in epitaxial $NdNiO_3$ thin films grown on $LaAlO_3$ substrates .

[1] S. Middey, et al. Annual Review of Materials Research, 46 (2016): 305-334.
[2] G. Catalan. Phase Transitions, 81 (2008): 729-749.
[3] S. Catalano, et al. Reports on Progress in Physics, 81 (2018): 046501.
[4] R. Jaramillo et al. Nature Physics, 10 (2014): 304-307.
[5] E. Mekheev etal. Science Advances 1 (2015): e150079706.
[6] D. Preziosi, et al. AIP Advances 7 (2017): 015210.

Multiferroic properties of coherently grown orthorhombic $R\mathrm{MnO_3}$ (R = Gd-Lu) thin films

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In this presentation, we will give an overview of the magneto-electric properties of a series of orthorhombic RMnO3 (R = Gd-Lu) thin films, coherently grown on (010) $YAlO_3$ substrates. The combination of chemical pressure and epitaxial growth is changing the b-axis lattice parameter while fixing the in-plane lattice constants. As a result, all coherently grown films show electrical polarization values up to $1\mu C/cm^2$ along the a-axis and T_{FE} is raised close to T_N. The induced strain also modifies the magnetic ground state of these materials. As measured by neutron and x-ray diffraction, the entire series shows a commensurate E-type antiferromagnetic order as a common ground state consistent with the relatively large spontaneous polarization. Our results further indicate, that the asymmetric Dzyaloshinski-Moria interaction in o-$R\mathrm{MnO_3}$ (R = Gd-Dy) is transformed by epitaxial strain into the symmetric exchange striction as the dominant mechanism for ferroelectricity.

Tailoring 'trapped' electrons in Ferroelectric Field Effect Devices

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Ferroelectric field effect devices (FeFEDs) rely on the non-volatile electric field generated onto the channel material by an adjacent ferroelectric layer[1]. As a genuine interfacial effect a measurable change in the functional properties of the channel material can be obtained only at extremely low thickness values. Recent studies on prototypical manganite-based FeFEDs[2] have shown that the pure electrostatic doping of charge carriers can effectively affect the magneto-transport properties of the (La,Sr)MnO3 channel material between the two stable and opposite polarization states at which, indeed, correspond an accumulation and/or depletion of charge carriers.
Here, for this poster presentation, the effect of a partial and increasing switching of the ferroelectric polarization via dedicate electrical pulses on the transport properties of a 4nm thick ferromagnetic $La_{0.825}Sr_{0.175}MnO_3$ thin film will be discussed. The perovskite $Pb(Zr,Ti)O_3$is used as ferroelectric gate. The heterostructures are grown via pulsed laser deposition by means of an AlO_x sacrificial layer shaped as Hall Bar geometry onto different substrates. At relatively low temperatures the observed upturn of the resistivity, which can most likely be associated to localization effects triggered by a combination of strain and dimensionality effects, is practically independent from the gradient of the electrostatic doping, while the slope of the resistivity curves change dramatically. Mott variable range hopping is used to fit the observed variation from which, by assuming for sake of simplicity, a constant localization length for all the intermediate polarization states, an increase of density of states at the Fermi level is observed from the depletion towards the accumulation state, as indeed expected. An out-of-plane applied magnetic field, on the contrary, is found to shift the temperature of such upturn, hence, bringing to a magnetic-induced localization state. The creation and/or increase in volume of ferromagnetic insulating domains which, affect the percolation pattern, is discussed in term of an effective modulation of the localization length of the 'trapped' electrons.

[1] P. M. Heyman, G. H. Heilmeier, Proc. IEEE 1966, 54, 842.
[2] D. Preziosi, I. Fina, E. Pippel, D. Hesse, X. Marti, F. Bern, M. Ziese, M. Alexe, Phys. Rev. B 2014, 90, 125155.

Ferroelectric field effect transistor based on $BaSnO_3$

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In order to integrate the newly discovered high-mobility perovskite semiconductor BaSnO3 [1] with a ferroelectric perovskite, we have grown epitaxial ferroelectric Pb(Zr,Ti)O3 (PZT) on 4 percent La-doped BaSnO3 (BLSO) and SrRuO3 (SRO) electrodes by pulsed laser deposition technique. X-ray diffraction measurement confirms that the PZT films were epitaxially grown and shows that the lattice constants of PZT depend on the Zr/(Zr+Ti) ratio in PZT. An all-epitaxial sandwich PZT ferroelectric capacitor structure was fabricated with BLSO and SRO electrodes, and the strain effect on the ferroelectric properties of PZT was investigated. The polarization-electric field (P-E) hysteresis curve is discussed from the viewpoint of the strain effect. Furthermore, ferroelectric field effect transistors with a BaSnO3 channel layer were successfully fabricated, and carrier modulation of BaSnO3 by the ferroelectric polarization field was observed. The output characteristics, the transfer characteristics and the breakdown field of the ferroelectric transistor will be presented.

[1] H. J. Kim, U. Kim et al., Appl. Phys. Express 5, 061102 (2012).

Local and correlated studies of humidity-mediated ferroelectric thin film surface charge dynamics

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Surface water is present on all materials exposed to ambient environmental conditions, inherently modifying the ground state in fundamental studies as well as affecting the operation of bare-chip devices. By virtue of its polar nature, water strongly interacts with domains and domain walls in ferroelectric materials: it influences polarisation switching dynamics in Pb(Zr0.2Ti0.8)O3 (PZT) thin films [1], and plays a key role (together with redistribution of oxygen vacancies) in the reversible control of electrical transport at 180° domain walls in this material [2].

Such water-polar surface interactions can be probed at the nanoscale by functional scanning probe microscopy (SPM), and analysed within the framework of unsupervised machine learning matrix factorization [3]. Here, we present our studies of the interaction of adsorbed water with written ferroelectric domains in thin films of PZT by Kelvin probe force microscopy imaging. Both the effect of polarization on the adsorbed water behaviour and the influence of surface water on the underlying material are investigated. Correlating the results of domains written with positive and negative tip voltage with the as-grown state of the film, we demonstrate changes in the strength of the electrostatic interactions between the SPM tip and the surface as a function of relative humidity and time. Statistical analysis performed on the acquired data sets suggests that the observed response is a combination of two competing physical behaviours: a fast materials-dependent process and a slower effect of polarization history. More in-depth scrutiny reveals spatiotemporal correlations invisible to the naked eye through the use of unsupervised machine learning techniques such as principal component analysis and dictionary learning.

[1] C. Blaser and P. Paruch, New J. Phys. 17, 013002(2015)

[2] I. Gaponenko, P. Tückmantel, J. Karthik, L. W. Martin and P. Paruch, Appl. Phys. Lett. 106, 162902 (2015)

[3] A. Belianinov, R. Vasudevan, E. Strelcov, C. Steed, S.M. Yang, A. Tselev, S. Jesse, M. Biegalski, G. Shipman, C. Symons, A. Borisevich, R. Archibald and S. Kalinin, Adv. Struct. Chem. Imag. 1, 6 (2015)

Imaging and modifying antiferromagnetic configurations in $BiFeO_3$

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Antiferromagnets are mainly useful in spintronics through their exchange bias properties, i.e. their ability to generate an effective field at the interface with a ferromagnet. In recent times, it has been realized that these materials can present several properties directly linked to their magnetic order. In particular, a large current density can influence the antiferromagnetic domains of some low-symmetry conducting compounds, in virtue of the effect of a staggered spin-orbit torque. So far, insulators, despite constituting the majority of magnetically ordered materials, have not been the object of much attention but their dynamical properties in the THz range are potentially of huge interest. Moreover, some of these present interesting multifunctional properties, which could be used to couple the antiferromagnetic order to another order parameter.

We will show here that indeed, magneto-electric coupling in the archetype multiferroic antiferromagnet BiFeO3 offers opportunities to control the antiferromagnetic order. As the effects work at room temperature, they allow a potential multifunctional memory device to be envisioned. Moreover, using strain engineering in films grown on different substrates one can produce samples where the AF order is cycloidal, as in the bulk, or homogeneous. In all cases, imaging the domain topography is an essential task but difficult to achieve because of the intrinsic AF magnetic compensation. We show here that using three techniques including NV-centre magnetometry [1], second harmonic light generation [2], and synchrotron diffraction it is possible to probe and image the AF order with submicron resolution, in both cycloidal and homogeneous forms. The magnetoelectric coupling can thus be visualised and different procedures involving applied electric fields, either DC or using a femtosecond light pulse, demonstrate that the AF domains can be modified independently of the electric polarization. This sub-coercive use of the magnetoelectric effect could open the door to memory devices where the information is purely antiferromagnetic.

[1] Real-space imaging of non-collinear antiferromagnetic order with a single spin magnetometer, I. Gross, W. Akhtar, V. Garcia, L. J. Martinez, S. Chouaieb, K. Garcia, C. Carrétéro, A. Barthélémy, P. Appel, P. Maletinsky, J.-V. Kim, J. Y. Chauleau, N. Jaouen, M. Viret, M. Bibes, S. Fusil and V. Jacques, Nature 549, 252 (2017).

[2] Multi-stimuli manipulation of antiferromagnetic domains assessed by second harmonic imaging, J.-Y. Chauleau, E. Haltz, C. Carrétéro, S. Fusil and M. Viret, Nature Materials 16, 803 (2017).

Ferroelectric fatigue of $PbZr_{0.52}Ti_{0.48}O_3$ epitaxial thin films: from cause and mechanism to strategies to avoid

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Ferroelectric fatigue, i.e. the reduction of the remnant polarization of ferroelectrics upon repeated polarization switching, causes an unstable and inefficient performance of ferroelectric devices. In the case of epitaxial, ferroelectric thin films, the fatigue behavior is mainly attributed to the effect of interfaces between the electrode and ferroelectric layers. Devices with metal electrodes show an extremely strong fatigue behavior, whereas capacitor structures with conducting oxide electrodes (e.g. $SrRuO_3$ (SRO)) possess an excellent fatigue endurance. Despite extensive investigations the origins and mechanisms of the ferroelectric fatigue still remain controversial [1].
In this work we used $PbZr_{0.52}Ti_{0.48}O_3$ (PZT) epitaxial thin films, grown by pulsed laser deposition (PLD) on a SRO bottom electrode and on $SrTiO_3$ substrate, as a model system to identify and clarify the origin and mechanism of ferroelectric fatigue. We directly observed structural phase degradation in an ultra-thin layer of PZT underneath the Pt top electrode in Pt/PZT/SRO structures upon electric pulse cycling, but not after the application of (high) dc bias field. This appears to be in accordance with a modelassuming that an initially imperfect interface (here between Pt and PZT) is the origin of the fatigue, giving rise to a very strong local depolarization field close to the Pt/PZT interface [2]. This in turn causes a high injected charge current into the ferroelectrics layer upon each polarization switch. This injection current locally generates sufficient heat to decompose over time the surrounding material, leading to the growth of passive, non-functional PZT areas nearby the interface with the Pt electrode. We propose that this blocking of the polarization switching is either caused by electric field screening by the growing thin dielectric layer or by trapping of charge in the interfacial passive layer. The local electric field induced by these trapped charges will prevent nearby polarization domains from switching. Based on the proposed model, we demonstrate that by either using an interfacial (conducting) oxide buffer layer or in situ deposition of metal electrode layers by PLD instead of a conventional sputtering step, the fatigue endurance of the structure can be significantly improved.

[1] 1 A.K. Tagantsev, I. Stolichnov, E.L. Colla, and N. Setter, J. Appl. Phys. 90, 1387 (2001).
[2] 2 X.J. Lou, M. Zhang, S.A.T. Redfern, and J.F. Scott, Phys. Rev. B 75, (2007).

Employing in-situ Frequency Dependent X-ray Scattering to Explore the Microscopic Response of Electrically Driven Epitaxial Strained and Free Membrane PMN-30PT thin films at the Morphotropic Phase Boundary.

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Bulk single crystal relaxor ferroelectrics such as 0.7Pb(Mg1/3Nb2/3)O3-0.3PbTiO3 (PMN-PT) have giant piezoresponses near their morphotropic phase boundary (MPB) compositions due to the rotation of internal polarization, leading to a field-induced phase transition from rhombohedral through monoclinic to tetragonal symmetries. The changes in mechanical and electrical boundary conditions that accompany device miniaturization can significantly affect the behavior of such a transition. Employing in situ synchrotron x-ray diffraction with an applied AC electric field, we first investigated the nature of this field-induced phase transition in fully strained ferroelectric PMN-PT epitaxial thin film heterostructures on silicon substrates at the rhombohedral side of the MPB. This talk will illustrate the reversibility between rhombohedral and monoclinic phases and how the transition demonstrates a strong frequency dependence. Between 1-10 kHz, an R to MA transition occurs while at higher frequencies (100kHz), an R - MB transition arises. The lattice response to electric field of both the R and monoclinic phases illustrates a strong elastic coupling behavior and the emergent phase seemingly drives the polarization switching process. Phase-field simulations and thermodynamic calculations describe the multi-phase microstructure mapping the likely polarization pathway of the transition itself.

In addition we employed a stroboscopic diffraction contrast imaging approach to study the spatial evolution traversing the 'free' membrane film. The underlying microscopic physical machinations of the morphotropic domain regime is difficult to intricately understand due to the instability of this mixed boundary phase. Here I will describe the approach developed to study the spatial dependent evolution of the symmetry across the transition itself. We have captured stroboscopic-like images mapping the intricate nature of the transition. Having fabricated free standing 0.7PMN-0.3PT thin film heterostructures patterned devices, which by driving a series of PE (partial) minor loops to continuously and in a controlled manner nucleate and grow the emerging symmetries mitigating the MPB transition process. Employing diffraction contrast imaging the lateral boundary condition defined by inactive material allows us to visually present the strain dependence upon the different components of the dynamic MPB transition.

By combining frequency modulated dynamic x-ray scattering with contrast imaging we have developed a powerful tool to intricately observe the spatial evolution of multiple parameters in-situ and concurrently.

Antiferroelectrics: flexoelectric and electrocaloric response

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Antiferroelectric materials are characterized by a spontaneous zero net polarization that can be switched into a ferroelectric state with an external electric field. Moreover, their dielectric constant undergoes a Curie-like anomaly at the phase transition, where it increases sharply. They have not being as researched as their ferroelectric counterparts, partly due to their centrosymetric and non-polar ground state, which make them less obvious for applications. Here we present experimental results on the anomalous electrocaloric and flexoelectric responses of these materials.

The electrocaloric response of antiferroelectrics has been researched due to their anomalous (negative) response, in which the samples decrease their temperature when a voltage pulse is applied. We have examined the response close to and beyond their Curie temperature, where we measured the negative-to-positive electrocaloric transition response with an infrared camera. Meanwhile, flexoelectricity- the coupling between polarization and strain gradient- is a universal property of all materials, but it has never been experimentally characterized in antiferroelectrics. And, yet, it has been hypothesized that the antiferroelectric phase might be stabilized by the influence of flexocoupling on the free energy of the system, thus pointing into a higher flexocoupling value than their ferroelectric or non-polar counterparts with the same lattice structure. We show that this flexocoupling is not higher than in simple dielectrics; however, unexpectedly, this flexocoupling is not constant as a function of temperature but increases sharply at the antiferroelectric-paraelectric phase transition.

Imaging Polarization Topologies in $BaTiO_3/SrTiO_3$ Superlattices

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In ferroelectric superlattices (SPLs), the electrostatic boundary conditions have a radical effect on the electric dipoles in the ferroelectric and can also induce formation of dipolar moments in the paraelectric. The recent observation of an unexpected vortex-like ferroelectric domain topologies in $PbTiO_3/SrTiO_3$ ferroelectric superlattices [1] has generated huge interest. In contrast, the dipoles distribution in $BaTiO_3/SrTiO_3$ superlattices has been far less investigated.
We have addressed this objective with a systematic characterization of symmetric n-$BaTiO_3$/n-$SrTiO_3$ SPLs, considering SPLs from short to large period (n=1, 2, 4 and 10 unit cells) [2]. For this we have used Aberration-Corrected Scanning Transmission Electron Microscopy (STEM) with picometer resolution in real space, which allows us to extract a map of polar distortions across the sample.
The results not only reveal a significant difference in the ferroelectric dipolar strength for different period SPLs, but also a remarkable variety of topologies formed by the collective arrangement of dipoles. Here, for the first time in $BaTiO_3$ SPLs, we were able to observe topologies such as flux closure rotations, waves and other more complex configurations. We compare these to some similar topologies recently observed in $PbTiO_3/SrTiO_3$ SPLs [3] and discuss how the different electrostatic conditions imposed by the SPLs period may lead to the formation of the different polar configurations. We also demonstrate the important role of O atoms in the formation of the polar configuration in $BaTiO_3/SrTiO_3$ SPLs, unveiling an unexpected different behaviour in $BaTiO_3$ and $SrTiO_3$ films.

[1] Yadav et al., Nature 530, 198 (2016)
[2] Khestanova et al., Ad. Funct. Mater. 26, 6446 (2016)
[3] Lu Lu et al., Physical Review Letters, 177601 (2018)

Selective control of multiple ferroelectric switching pathways using trailing flexoelectric field and its implications

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While conventionally manipulated by the electrical bias of a scanning probe, the polarization domain in ferroelectric thin films can also be reoriented by mechanical force through the tip by virtue of the flexoelectricity. Although the mechanical approach for polarization switching has been demonstrated in a number of ferroelectric materials, most investigations concern only the 180° reversal of the out-of-plane polarization[1]. However, a systematic study is still lacking for the domain switching in more complex situations where both non-180° ferroelastic and 180° ferroelectric switching coexist.

In ferroelectric materials, more than one polarization switching pathway can be an important ingredient for novel electronic devices, such as multilevel memory storage. Especially, if the ferroelectric materials possess other ferroic ordering, namely like multiferroic BiFeO3 (BFO), the multiple switching pathways can be utilized for magnetoelectric devices. However, for actual realization of those devices, deterministic control of multiple polarization switching pathways is an essential prerequisite. Although there were many efforts to selectively control the ferroelectric switching pathways and several studies have shown its possibility, typically they required additional laborious processes[2,3].

In our work, we show that as a new non-electrical approach, 'trailing flexoelectric field' offers a simple but very effective route for selective control of multiple ferroelectric switching pathways in a BFO thin film[4]. The simple pressing of the electrically grounded SPM tip and the control of its motion allow us to select particular domain switching only. Also, we discuss the possible implications on how to exploit the trailing flexoelectric field.

[1] Lu, H. et al. Mechanical writing of ferroelectric polarization. Science 336, 59-61 (2012).

[2] Baek, S. H. et al. Ferroelastic switching for nanoscale non-volatile magnetoelectric devices. Nat. Mater. 9, 309-314 (2010).

[3] Morelli, A., et al. Deterministic Switching in Bismuth Ferrite Nanoislands. Nano Lett. 16, 5228-5234 (2016)

[4] Park, S. M. et al. Selective control of multiple ferroelectric switching pathways using trailing flexoelectric field. Nat. Nanotech. 13, 366-370 (2018)

Advanced Functional Testing of Oxide Electronic Systems

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Thin-piezoelectric-film and thin-ferroelectric-film technologies have matured to the point that commercial components are under consideration. It is also clear that the first oxide electronics are being integrated with piezoelectric and ferroelectric components leading to the possibility of standalone oxide IC circuits with embedded sensors divorced from dependence upon external silicon integrated circuits! Experimental examples have been published by Penn State and Radiant Technologies.[1,2] External control circuitry combined with electromechanical devices are required for such components (i) to be tested or (ii) to be deployed. The testing and evaluation environment for such products must efficiently control external electronics, thermal chambers, and electromechanical relays in addition to conducting classic non-linear materials measurements. In this study, we propose a new testing concept that combines digital and analog function generation along with the rich capabilities of a modern ferroelectric looper into a single framework. The integrated test environment for such systems-on-chip must also be able to characterize non-linear transistors.

Our technique combines all of the hardware and software functions necessary to characterize fully integrated oxide systems-on-chip. In order to verify the testing procedures, and explore possible commercial applications, we fabricated and tested in-house a wide range of fully integrated and packaged thin-PZT-film components including ferroelectric capacitors, piezoMEMS, thin ferroelectric film transistors (TFFTs), and thin ferroelectric film diodes, all made from heterostructures of thin oxides and metals. Results show that a single test framework (we call 'piezoMEMS Analyzer') can measure ferroelectric and piezoelectric films, perform classical systems analysis, communicate with electronic circuitry (whether oxide or classical silicon), and control environmental chambers, all from a single user interface. Thus the piezoMEMS Analyzer framework serves as an Autonomous Automated Test Environment for oxide electronics research.

[1] J.I. Ramirez, "ZnO Thin Film Electronics for More than Displays", Dissertation for a Doctor of Philosophy in Electrical Engineering, Pennsylvania State University, August 2015 https://etda.libraries.psu.edu/files/final_submissi
[2] J Evans, "Technical Report - MFIS and TFFT Testing with the Premier II Tester", Radiant Technologies, Inc, September 2011, https://www.ferrodevices.com/1/297/files/ApplicationNote-FerroelectricTransistorTesting.pdf

Direct tunneling and capacitance spectroscopy in Au - $(LaAlO_3)_4$ - $SrTiO_3$ tunnel junctions

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The energy spectrum of a quasi-two-dimensional electron system (q-2DES) can be probed using perpendicular tunneling spectroscopy. This was done for the intensively studied $LaAlO_3$-$SrTiO_3$ interface to reveal an unconventional dependence of the superconducting gap on gate voltage [1]. A follow-up study investigated electron-phonon coupling through the corresponding inelastic tunneling spectrum [2]. Here, we perform tunneling experiments using Au tunnel electrodes grown in situ by pulsed laser deposition, suppressing the total current density by several orders of magnitude. The current is almost independent of temperature, which shows that our devices exhibit a very pure, direct tunneling current with very minute ohmic contributions through defect states.
Analysis of the normalized differential conductance (NDC) across the junction at 10 mK suggests that the Fermi level of the q-2DES is located about 50 meV below the bulk conduction band edge. By applying a backgate voltage across the $SrTiO_3$ substrate, in the range of -25 V to +25 V, we did not observe a superconducting gap nor a supercurrent, which suggests that the carrier density at the interface is very high [1]. With backgate voltage, robust and small features start to move, which upon analysis appear unrelated to the quantum well states. We ascribe them to tunneling through a small number of well-defined defect states in the $LaAlO_3$ barrier.
Besides dc tunneling measurements, we performed frequency-dependent transport measurements across the junction. By using a very simple equivalent circuit, we extracted the device capacitance as function of dc bias across the junction and of backgate voltage. The measurement results suggest that the capacitance depends primarily on the total carrier density, and saturates for high density, in accordance with previous results [3]. In the region of negative bias and positive backgate voltage, we measure a slight enhancement of the capacitance, implying negative compressibility. We propose that this indication of a thermodynamic instability is due to the electrostatic boundary conditions for the confining potential well.
Our results imply firstly that our fabrication method results in excellent complex oxide tunnel junctions and field effect devices with an ultrathin insulating barrier. In our transport measurements, we observe several features that were previously unobservable due to large leakage currents hindering both the direct tunneling measurement and the capacitance measurement. We foresee that exploration of similar devices with lower carrier density, especially in the direction of superconductivity, could lay bare the fundamental physics underlying the phenomenology of the interface.

[1] C. Richter et al., Nature 502, 548 (2013)
[2] H. Boschker et al., Scientific Reports 5, 12309 (2015)
[3] L. Li et al., Science 332, 825 (2011)

Large positive linear magnetoresistance in the two-dimensional t_{2g} electron gas at the EuO/$SrTiO_3$ interface

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The high mobility two-dimensional t_{2g} electron gas (2DEG) present at oxide/oxide interfaces is currently under intense investigation [1-2]. In this talk, we will discuss the integration of highly spin-split ferromagnetic semiconductor EuO onto perovskite $SrTiO_3$ (001). A careful deposition of Eu metal by molecular beam epitaxy results in crystalline EuO growth via oxygen out-diffusion from $SrTiO_3$ [3]. This in turn leaves behind a highly conductive interfacial layer through generation of oxygen vacancies. Below the Curie temperature of 70 K of EuO, this spin-polarized two-dimensional t_{2g} electron gas at the EuO/$SrTiO_3$ interface displays very large positive linear magnetoresistance (MR). Soft X-ray angle-resolved photoemission spectroscopy (SX-ARPES) reveals the t_{2g} nature of the carriers. First principles calculations strongly suggest that Zeeman splitting, caused by proximity magnetism and oxygen vacancies in $SrTiO_3$, is responsible for the MR [4]. This system offers an as-yet-unexplored route to pursue proximity-induced effects in the oxide two-dimensional t_{2g} electron gas [5].

[1] J. K Lee, N. Sai, and A. A. Demkov, "Spin-polarized 2DEG through electrostatic doping in $LaAlO_3$-EuO heterostructures", Phys. Rev. B **82**, 235305 (2010).

[2] K. D. Fredrickson and A. A. Demkov, "Spin-polarized, orbital-selected hole gas at the EuO/Pt interface," J. Appl. Phys. **119**, 095309 (2016).

[3] A. B. Posadas, K. J. Kormondy, W. Guo, P. Ponath, J. Geler-Kremer, T. Hadamek, and A. A. Demkov, "Scavenging of oxygen from $SrTiO_3$ during oxide thin film deposition and the formation of interfacial 2DEGs," J. Appl. Phys. **121**, 105302 (2017).

[4] L. Gao and A. A. Demkov, "Spin-polarized two-dimensional t_{2g} electron gas: Ab initio study of EuO interface with oxygen-deficient $SrTiO_3$," Phys. Rev. B **97**, 125305 (2018).

[5] K. J. Kormondy, L. Gao, X. Li, S. Lu, A. B. Posadas, S. Shen, M. Tsoi, M. R. McCartney, D. J. Smith, J. Zhou, L. L. Lev, M. Husanu, V. N. Strocov, and A. A. Demkov, "Large positive linear magnetoresistance in the two-dimensional t_{2g} electron gas at the EuO/$SrTiO_3$ interface," Scientific Reports (2108) doi: 10.1038/s41598-018-26017-z

Coupled Cu- and Mn charge and orbital orders in cuprate/manganite

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The observation of a charge density wave in the underdoped cuprate high Tc superconductors (Cu-CDW)has raised a debate about its relationship with superconductivity [1-3]. In $YBa_2Cu_3O_{7-\delta}$ (YBCO) single crystals the Cu-CDW appears to be incipient and mainly pinned by defects [4]. Nevertheless, a large magnetic field induces a true long-range CDW order as it suppresses superconductivity [5, 6]. An enhanced Cu-CDW order was also observed in $YBa_2Cu_3O_7/La_{2/3}Ca_{1/3}MnO_3$ (LCMO) multilayers [7,8]. Here, we show that the magnitude of the induced Cu-CDW in cuprate/manganite multilayers can be varied by adjusting the strength of the charge and orbital order in the manganite (Mn-COO). This is achieved with $Nd_{0.65}(Ca_{1-y}Sr_y)_{0.35}MnO_3$ (NCSMO) layers for which the Mn-COO can be readily tuned via the Sr content through the control of the tolerance factor. This provides unique opportunities to study the relationship between the Cu-CDW and superconductivity and can even lead to new coupled quantum states.

[1] Wu, T. et al., Nature **477**, 191-194, (2011).
[2] Ghiringhelli, G. et al., Science **337**, 821, (2012).
[3] Chang, J. et al., Nat. Phys. **8**, 871-876, (2012).
[4] Wu, T. et al., Nat. Commun. **6**, 6438, (2015).
[5] Chang, J. et al., Nat. Commun. **7**, 11494, (2016).
[6] Gerber, S. et al., Science **350**, 949, (2015).
[7] Frano, A. et al., Nat. Mater. **15**, 831-834, (2016).
[8] He et al., Nat. Communications **7**, 10852 (2016).

Oxygen-vacancy-assisted recovery process for increasing electron mobility in n-type $BaSnO_3$ epitaxial thin films

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New transparent oxide semiconductors (TOSs) have received extensive interests and demands for the application of current optoelectronic devices. In particular, La-doped $BaSnO_3$ (LBSO) have recently attracted much attention due to the excellent room-temperature (RT) electron mobility (μ 320 $cm^2V^{-1}s^{-1}$ at $n = 8.0\ 10^{19}$ cm^{-3} in a single crystal) and the excellent thermal stability [1]. Despite the great potential of LBSO for transparent electronics, epitaxial LBSO films were reported to show much lower electron mobility than single crystals, which has been ascribed into the high density of line defects, i.e., dislocations, which are generated by lattice mismatch between substrate and film [2].
In this research, we demonstrate the significant increase in the room-temperature electron mobility of LBSO by delicately modulating the oxygen vacancy (V_O) concentration by post-growth treatment. Through the accurate adjustment of oxygen partial pressure (pO_2) under annealing, the room-temperature mobility of LBSO films on STO substrates could increase up to 115 $cm^2V^{-1}s^{-1}$ at a carrier concentration of 1.2×10^{20} cm^{-3}, which results in simultaneous increase of carrier density and mobility [3]. The electrical, optical and structural effects of V_O formed during annealing were systematically investigated, and especially, significant reduction of threading dislocations was directly observed by bright-field and dark-field image of transmission electron microscopy and reciprocal space mapping of x-ray diffraction. Thus, the enhancement of RT electron mobility by adjusting pO_2 was attributed to the annihilation of threading dislocation by high-temperature recovery process, i.e., the dislocation annihilation through oxygen-vacancy-induced climb. Our finding suggests that the interaction between point defects and line defects can be exploited to boost carrier density and mobility in transparent oxide semiconductors.

[1] Annu. Rev. Mater. Res. 47, 391-423 (2017)
[2] Applied Physics Express 5, 061102 (2012)
[3] NPG Asis Materials, advance online publication (2018) (doi:10.1038/s41427-018-0038-1)

2-dimensional electron gas oxide remote doping of Si(001)

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2-dimension electron gas (2DEG) oxide heterostructures based on rare earth titanates have been shown to support high electron densities, but devices fabricated from such structures have limited room temperature electron mobilities. We demonstrate the integration of a 2DEG oxide structure comprised of $LaTiO_3/SrTiO_3$ (LTO/STO) on undoped Si(001) that possesses the attractive attributes of high charge density from the oxide and high mobility of silicon. Key to this approach is modification of the oxygen content at the STO-Si interface, which tunes the band alignment and induces electron carriers to move from the oxide 2DEG to form a 2DEG in the silicon substrate. We confirm the shift of the STO-Si conduction band by x-ray photoelectron spectroscopy measurements and quantify the conduction in the heterostructure with a two channel Hall model. As a consequence of a reduced band offset between STO and Si, the overall mobility of the heterostructure increases by two orders of magnitude compared to that in the oxide 2DEG to up to 100 $cm^2V^{-1}s^{-1}$ at room temperature, with a carrier density of 1×10^{13} cm^{-2}. This approach can be applied to technologies that require both high carrier and high carrier mobility for applications in plasmonics and high power electronics, and also demonstrates an example of combining multifunctional complex oxides with conventional semiconductors.

Two-Dimensional Electron Gases at the (111) - Surfaces of $KTaO_3$ and $SrTiO_3$

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Two-dimensional electron gases (2DEGs) in oxides are among the major building blocks in the field of oxide electronics. The possibility of enhancing the functional properties of oxides in confined geometries, together with the opportunity to tune such properties, for example by field effect modulation of carrier density, is very attractive. Recently, it was observed that an interface-driven spin-orbit coupling mechanism, the Rashba effect, can be used in oxide 2DEGs to achieve very efficient spin-to-charge conversion. This has renewed interest in detailed studies in the electronic structure of oxide 2DEGs. In this work we report direct measurements of the electronic band structure of the 2DEG stabilized in (111)-oriented surfaces of $KTaO_3$ (KTO) and $SrTiO_3$ (STO) crystals using angle resolved photoemission spectroscopy (ARPES). Our tight-binding supercell calculations based on relativistic density functional theory calculations of the bulk band structure are in good agreement with the experimentally found six-fold symmetric Fermi surfaces in both systems. Remarkably, we find that the in-plane Rashba spin splitting is of similar magnitude in both systems despite the dramatic difference in atomic spin-orbit coupling between KTO and STO. Our calculations allow us to examine the details of the spin and orbital texture of these (111) orientated 2DEGs. We reveal a previously unreported and significant out-of-plane spin component for the subbands of the STO and KTO (111) 2DEGs which has only three-fold rotational symmetry. We confirmed the presence of this momentum dependent out-of-plane spin component by measuring the bilinear magnetoelectric resistance (BMER) effect in STO (111) 2DEGs.

[1] Phys. Rev. Lett 113, 177601 (2014)

Photoresponse dynamics and photoconductivity mapping in $LaAlO_3/SrTiO_3$ interfaces

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Despite the insulating character of the constituent materials, a highly-conductive 2D-electron gas develops across a nm-thick region around the $LaAlO_3/SrTiO_3$ interface [1]. This 2DEG hosts a number of properties, including magnetism, 2D-superconductivity, and large Rashba spin-orbit fields. Less explored, although not less interesting, is the fact that these systems show persistent photoconductance (PPC), by which the conductance of the interface suddenly increases after visible (or ultraviolet) light illumination [2]. The effect persists after switching off light, and the initial resistivity is not recovered over long periods of time, from minutes to many hours.
For any technological development it is crucial to understand the dynamic response of the photoconductance. For that purpose, we have investigated the time dependence of photo-induced changes in the conductance triggered by light pulses in the visible spanning a wide range of timescales, from seconds down to tens of microsecond [3]. For the purpose of our study, we designed Hall-bar devices with micron-sized lengths defined by optical lithography and performed electrical measurements by illuminating the samples in-situ with light of different wavelengths using a scanning confocal microscope, which enabled us to map out the photoconductance with diffraction-limited resolution. Based on these experiments, we analysed the dynamic response (rise and decay times) in terms of stretched exponential functions, which allowed us to determine the activation energy spectrum under the inverse Laplace transform method. Our results are compatible with a mid-gap state model, by which PPC requires charges to be trapped in long-life metastable states that prevent the recombination of electron-hole pairs created by photons. The mechanism relies on the existence of defects which are bistable between a shallow and a deep energy state that swap into one another by the action of photons changing their occupancy. Our results provide important information for the development of prospecting applications based on PPC, including holographic data storage or photonic neuromorphic networks.

[1] Ohtomo, Hwang, Nature 427, 423 (2004).
[2] Tebano et al., ACS Nano 6, 12787 (2012).
[3] Y. Chen et al., in preparation.

Charge doping and large lattice expansion in oxygen-deficient heteroepitaxial WO_3

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Tungsten trioxide (WO_3) is a versatile material with widespread applications ranging from electrochromics and optoelectronics to water splitting and catalysis of chemical reactions. For technological applications, thin films of WO_3 are particularly appealing, taking advantage from a high surface-to-volume ratio and tunable physical properties. However, the growth of stoichiometric crystalline thin films is challenging because the deposition conditions are very sensitive to the formation of oxygen vacancies. In this talk, I will show how background oxygen pressure during pulsed laser deposition can be used to tune the structural and electronic properties of WO_3 thin films. By performing X-ray diffraction and low-temperature electrical transport measurements, we find changes in the WO_3 lattice volume of up to 10% concomitantly with a resistivity drop of more than five orders of magnitude at room temperature as a function of increased oxygen deficiency. We use advanced *ab initio* calculations to describe in detail the properties of the oxygen vacancy defect states and their evolution in terms of excess charge concentration. Our results depict an intriguing scenario where structural, electronic, optical, and transport properties of WO_3 single-crystal thin films can all be purposely tuned by controlling the oxygen vacancy formation during growth.

[1] G. Mattoni, et al., Phys. Rev. Materials 2, 053402 (2018)

Ionic Liquid Gating of $SrIrO_3$ Ultra-Thin Films

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Perovskite $SrIrO_3$ (SIO) is a narrow-band semimetal, which combines strong spin-orbit coupling and electron correlations. This system has attracted much attention because it is at the verge of a Mott transition [1] and a ferromagnetic instability [2]. In epitaxial SIO ultra-thin-layers, a thickness dependent metal-insulator transition (MIT)has been observed [3]. It has been explained in terms of the opening of a Mott gap. At the moment it is not clear whether the transition is band-width or carrier-density-controlled. In this work we have explored MIT in SIO ultrathin-layers by using Electric Double Layer (EDL) techniques, that employ ionic liquid as gate dielectric. This technique is used to modify the carrier up to extremely high concentrations, at the level of an electron per formula unit, that can stabilize novel phases in strongly-correlated systems. We have simultaneously measured longitudinal (magneto) resistance and Hall effect across this transition. Increasing the doping at the highest level, we are not only able to modify the transition temperature, but also to reach an insulating state which exhibits a strong temperature dependence of the resistance , hysteretic-magnetoresistance and anomalous Hall effect at low temperature, suggesting ferromagnetic order.

[1] [1] Y. F. Nie, P. D. C. King, C. H. Kim, M. Uchida, H. I. Wei, B. D. Faeth, J. P. Ruf, J. P. C. Ruff, L. Xie, X. Pan et al., Phys. Rev. Lett. 114, 016401 (2015)
[2] [2] G. Cao, V. Durairaj, S. Chikara, L. E. DeLong, S. Parkin, and P. Schlottmann Phys. Rev. B 76, 100402(R)
[3] [3] D. J. Groenendijk, C. Autieri, J. Girovsky, M. C. Martinez-Velarte, N. Manca, G. Mattoni, A. M. R. V. L. Monteiro, N. Gauquelin, J. Verbeeck, A. F. Otte, M. Gabay, S. Picozzi, and A. D. Caviglia, Phys. Rev. Lett. 119, 256403 (2017)

The fabrication of s-wave/p-wave superconducting oxide heterojunctions

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The interfacial coupling of s-wave spin singlet superconductor (SSC) and p-wave spin triplet superconductor (TSC) can provide a variety of intriguing physics related to proximity effect of orbital parity. C. Honerkamp *et al.* predicted the Josephson critical current (I_c) would show extraordinary behavior at the SSC/TSC/SSC junction, due to opposite phase between two s-wave superconductors. R. Jin *et al.* fabricated Pb/Sr_2RuO_4/Pb Josephson junction, and seemed to realize the theory of s-wave/p-wave Cooper pair mixing effect. However, T. Nakamura *et al.* revealed that the result of Pb/Sr_2RuO_4/Pb Josephson junction comes from its intrinsic topological physics, not from superconducting proximity effect. The s-wave/p-wave Cooper pair proximity effect was disturbed by the atomic structures at Pb/Sr_2RuO_4 interface, such as oxide insulating layers or metallic Ru lamellae. Hence, improving the interfacial quality of the Josephson junction is crucial to get deeper understanding of the interfacial coupling of SSC and TSC.

Here, we propose a new SSC/TSC/SSC junction, by employing $BaPb_{1-x}Bi_xO_3$/Sr_2RuO_4 oxide heterostructure. $BaPb_{1-x}Bi_xO_3$ (BPBO) is oxide s-wave superconductor with bulk $T_c = 12\,\mathrm{K}$. This all-oxide junction is expected to show a atomically sharp interface and thus good device performance. To realize this heterojunction, we deposited BPBO thin films on cleaved Sr_2RuO_4 single crystal substrates by pulsed laser deposition technique. The epitaxial quality of BPBO film is confirmed by X-ray diffraction. Also, we confirmed the superconductivity of BPBO on Sr_2RuO_4 by Magnetic Property Measurement System. The device fabrication for BPBO/Sr_2RuO_4/BPBO junctions is done by photolithography and e-beam lithography technique. In the end, we will show the I_c of BPBO/Sr_2RuO_4/BPBO junctions by Physical
Property Measurement System.

[1] M. Sigrist *et al.*, Prog. Theo. Phys. **100**, 53 (1998).
[2] R. Jin *et al.*, Phys. Rev. B **59**, 4433 (1999).
[3] T. Nakamura *et al.*, Phys. Rev. B **84**, 060512 (2011).

Interface band engineering in $LaAlO_3/SrTiO_3$ heterostructures

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Novel two-dimensional electron systems at the interfaces of oxide heterostructures, as e.g. in $LaAlO_3/SrTiO_3$ (LAO/STO), recently have attracted much attention. A key requirement for future applications is the controllability of the electronic interface properties. We show that these properties can be controlled in LAO/STO by the oxygen vacancy (V_O) concentration which we adjust during photoemission experiments by means of synchrotron light irradiation and simultaneous oxygen dosing [1]. In detail, the V_O concentration determines the density of mobile and trapped charge carriers and consequently the band bending and alignment at the interface.

We systematically investigate these properties on (001) and (111) oriented LAO/STO heterostructures with controlled V_O concentrations through depth profiling of the film and substrate core levels by means of angle-dependent hard X-ray photoelectron spectroscopy. Fits using a self-consistent Poisson-Schrödinger ansatz yield a complete picture of the band alignment at the interface as a function of V_O concentration. We find, in particular, that the interfacial band profile is strongly affected by the electric field dependence of the STO dielectric constant.

[1] Phys. Rev. B 95, 195109 (2017)

Misfit Controlled Electrical Conductivity and Simultaneous Optimization of Carrier Density and Mobility in Transparent Metallic 3*d* Oxide Films

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Transparent conductors based on strongly correlated 3*d* metals are receiving much attention as they display a rare combination of having an electrical conductivity similar to that of noble metals (e.g. Pt) while having a plasma frequency in the near infrared region [1]. For instance, it has been shown that $SrVO_3$ thin films may display an outstanding room temperature resistivity as small as 20-40 $\mu\Omega$·cm [1-2]. However, it turns out that films properties are strongly dependent on processing conditions. For example, the growth window is extremely narrow and it has been reported [2] in MBE-grown films that, point defects related to cationic stoichiometry (i.e. Sr:V ratio) largely determine the film's conductance and residual resistivity ratio. However, it is not yet precisely known the role of point defects on carrier density and mobility. Here, to get a new insight into the role of misfit strain-related defects on the ultimate electrical conductivity and carrier mobility we explore the properties of $SrVO_3$ epitaxial films grown by PLD on substrates causing different misfit strain to modulate the microstructure and under different conditions to modulate carrier density.

We first show that the film's conductivity is enhanced when films are grown on substrates inducing minimal misfit strain. This observation holds irrespectively on the atmosphere (Ar, O_2 or vacuum) used during film growth, suggesting a dominating role of strain-relaxation related defects in the film microstructure governing the film conductance. Electron microscopy images indeed confirm this claim. Moreover, it is found that the carrier density and mobility of $SrVO_3$ films can be both modulated (increased) simultaneously (as observed in GaN films [3]). This is in evident contrast with the common decrease of mobility with increasing doping observed in semiconductors, including the much-used ITO ($Sn:In_2O_3$) transparent metallic oxide. We will next show that whereas $SrVO_3$ conductivity increases when reducing the oxygen pressure during growth a further optimization can be achieved by reducing the kinetic energy of the laser plasma plume species. By appropriate combination of substrate selection and PLD growth conditions, $SrVO_3$ films displaying a room temperature resistivity of around 30 $\mu\Omega$·cm, a record resistivity ratio in films grown by PLD, and a plasma frequency at 1.2 eV (1035 nm) can be obtained.

[1] L. Zhang et al., Nature Materials 15, 204-210 (2016)
[2] M. Brahlek et al., Applied Physics Letters 107, 143108 (2015)
[3] H.M. Ng et al., Applied Physics Letters 73, 821 (1998)

Seeing the birth of conductivity at oxide interfaces - an in-situ transport study

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Functional oxides stimulated a lot of research interest due to its variety of properties. As a major fabrication method for oxide thin films, Pulsed Laser Deposition (PLD) is routinely applied for creating SrTiO3 (STO) based heterostructures.

In the light of the vast phenomena present in these conducting interfaces, several studies focus on altering its properties after the deposition [1,2]. However, little is known about the process on how the conductivity forms during the pulsed laser deposition and the possibilities to tune the properties at this very first stage. This knowledge is typically acquired by characterizing the heterostructure ex situ after their fabrication.

Here we present in-situ transport studies of the interface, during deposition of LaAlO3, LaSrMnO3 and γ-Al2O3 on STO at room temperature. We measure the formation of the electron system during deposition, and relate it to various deposition conditions, while we also study the effect of photo-induced conductivity and separate photo- and particle effects by physical filters.

[1] 1. Hurand S et al. Field-effect control of superconductivity and Rashba spin-orbit cou-pling in top-gated LaAlO3/SrTiO3 devices. Scientific Reports (2015), 12751.

[2] 2. Christensen DV et al. Controlling the Carrier Density of SrTiO3-based Heterostruc-tures with Annealing. Advanced Electronic Materials (2017), 1700026.

Inducing magnetism in the electron gas at $LaAlO_3/GdTiO_3/SrTiO_3$ interfaces

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At the interface between band insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) a two-dimensional electron gas (2DEG) can be formed. There are also indications that the Ti^{3+} ions can give rise to (spurious) magnetism. However, fabricating a homogeneous spin-polarized electron gas is still a challenge. One strategy is to bring rare earth ions close to the interface. After inserting a 2-unit-cell layer of the band insulator $EuTiO_3$ (ETO) an anomalous Hall effect (AHE) was reported [1], as a signature for magnetism. In our work we inserted 2 unit cells of the Mott insulator $GdTiO_3$ (GTO) between LAO and STO. Note that the Eu-ion in ETO is divalent (like Sr), while the Gd-ion in GTO is trivalent (like La). Samples were prepared by Pulsed Laser Deposition. The temperature dependence of the sheet resistance shows that a 2DEG has formed. Gating the system at low temperatures with a negative voltage leads to a metal-insulator transition, with a Kondo like resistance minimum. For positive voltages, the system becomes increasingly metallic and shows an AHE as well as hysteretic behavior of Hall coefficient. We conclude that magnetism is induced, but only at finite gate voltages.

[1] Stornaiuolo, D. et al. Tunable spin polarization and superconductivity in engineered oxide interfaces. *Nat. Mater.* **15**, 278-283 (2016).

The Effect of $LaFeO_3$ Spacer Layer on Electrical Properties of $LaAlO_3/SrTiO_3$ Interfaces

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Introduction of spacer layer to modulate the properties of quasi two dimensional electron gas (q2DEG) formed at $LaAlO_3/SrTiO_3$ (LAO/STO) interfaces has been an interesting theme of research in recent periods, e.g. for mobility enhancement and spin polarization by introduction of $La_{1-x}Sr_xMnO3$ (LSMO)[1] and $EuTiO_3$ (ETO)[2], respectively. Along these lines, we have systematically studied the influence of delta doing $LaFeO_3$ (LFO) spacer layer on the q2DEG formed at crystalline and amorphous LAO/STO interface. By increasing the thickness of LFO (in u.c.), carrier density can be tuned by over two orders of magnitude accompanied by an enhancement in mobility. Critical thickness for metal-to-insulator transition (MIT) was found to be 2.35 nm (6 u.c.) and 1.17 nm for the crystalline and amorphous LAO/STO systems, respectively. XAS measurement indicated the creation of additional Fe^{2+} ions in LFO layers when charge transfer occurs. Transport measurements have also shown the formation of additional carrier scattering centers, which alters with the thickness of LFO. Our transport magnetoresistance measurement confirms the existence of spin-orbit interaction without the application of any external electric field. The observation shows the magnitude of the spin-orbit coupling can be enhanced with varying u.c. of LFO.

[1] Extreme mobility enhancement of two-dimensional electron gases at oxide interfaces by charge-transfer-induced modulation doping. Nature materials, 2015. 14(8): p. 801. 2. Stornaiuolo, D., et al., Tunable spin polarization and superconductivity in engineered oxide interfaces. Nature materials, 2016. 15(3): p. 278.
[2] Stornaiuolo, D., et al., Tunable spin polarization and superconductivity in engineered oxide interfaces. Nature materials, 2016. 15(3): p. 278.

Unconventional anomalous Hall effect in $SrRuO_3$ thin films

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The canonical metal oxide, $SrRuO_3$, is a 4d ferromagnet with a bulk Curie temperature, T_C, of 160K. Ferromagnetism in this system is supported by distortions of the oxygen octahedra that are coupled to a strong hybridization between O 2p and the Ru 4d orbitals. Thin films of $SrRuO_3$ on $SrTiO_3$ (100), on the other hand exhibit tunable physical properties including a metal-insulator transition, coexistence of ferromagnetic/antiferromagnetic/spin glass states and are thus quite different from the bulk. Magnetic anisotropy in $SrRuO_3$ thin films can also be tailored and are relatively complex. For thin films, the easy axis is usually in the out of the plane of the film surface and can be temperature dependent. Such interfaces have been found to host different topological spin textures aided by non collinear magnetic effects either at the interface with the substrate or with a capping layer.
In this work, strained $SrRuO_3$ thin films were epitaxially grown on $SrTiO_3$ (100) substrates by pulsed laser deposition (PLD). Magnetic and structural characterization establishes a perpendicular magnetic anisotropy in our thin films. We perform electrical transport measurements on our patterned films over a large temperature range. We observe an unconventional anomalous Hall effect in our films, different from those recently reported. We will present our analysis of the results considering the effects of dipolar coupling and exchange interaction at our tailored interfaces.

Superconductivity at $LaAlO_3$/Ca doped $SrTiO_3$ interfaces

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The superconducting state of doped $SrTiO_3$ is somehow unique since it appears at the lowest carrier concentration between the superconducting materials and is close to a ferroelectric order. Recent work has investigated the influence of ferroelectric fluctuations on superconductivity [1-3]. Theory predicts an enhancement of the superconducting transition temperature (T_c) for samples in the vicinity of the ferroelectric quantum critical point (QCP) [1]. Experimental studies in ferroelectric $SrTi^{18}O_{3-\delta}$[2] and $Sr_{1-x}Ca_xTiO_{3-\delta}$($0.002 < x < 0.02$) [3] have indeed revealed that, for the same value of carrier concentration, T_c is higher for ^{18}O and Ca-doped $SrTiO_3$ samples compared with $SrTiO_{3-\delta}$ samples.
In this study, we investigate superconductivity at $LaAlO_3/Sr_{1-x}Ca_xTiO_3$ interfaces (x = 0.0025, 0.005, 0.01, and 0.05) to clarify how the 2D electron liquid at the interface is affected by the ferroelectric QCP. A clear metallic behavior is observed in $LaAlO_3$ (10 u.c.)$/Sr_{1-x}Ca_xTiO_3$ (x = 0.025, 0.005 and 0.01) heterostructures. For $LaAlO_3/Sr_{1-x}Ca_xTiO_3$ (x = 0.005 and 0.01) interfaces, we observe a superconducting transition, but not for $LaAlO_3$/
$Sr_{1-x}Ca_xTiO_3$ (x = 0.0025 and 0.05). We will discuss the superconducting and magnetotransport properties of the $LaAlO_3/Sr_{1-x}Ca_xTiO_3$ (x = 0.005 and 0.01) interfacial system under field effect.

[1] J. M. Edge, Y. Kedem, U. Aschauer, N. A. Spaldin, and A. V. Balatsky, Quantum Critical Origin of the Superconducting Dome in SrTiO3, Phys. Rev. Lett., 115 (2015) 247002.
[2] A. Stucky, G. W. Scheerer, Z. Ren, D. Jaccard, J.-M. Poumirol, C. Barreteau, E. Giannini and D. van der Marel, Isotope effect in superconducting n-doped SrTiO3, Sci. Rep. 6 (2016) 37582.
[3] C. Rischau, X. Lin, Ch. P. Grams, D. Finck, S. Harms, J. Engelmayer, T. Lorenz, Y. Gallais, B. Fauqué, J. Hemberger and K. Behnia, A ferroelectric quantum phase transition inside the superconducting dome of Sr1-xCaxTiO3-d, Nat. Phys. 13, 643-648 (2017).

Electrolyte gating on high-Tc cuprates: superconductor-insulator phase transition and mechanism investigation

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Electrolyte gating is widely used to induce large carrier density modulation on solid surfaces to explore various properties. Here, we use electrolyte gating to tune the carrier density in an electron-doped cuprate Pr2-xCexCuO4 (PCCO) ultrathin film and cause a two-dimensional insulator-superconductor transition (SIT) at critical sheet resistances (Rc) much lower than the pair quantum resistance RQ=h/(2e)2=6.45 kΩ which is seen in hole-doped cuprate. The low upper critical field in this system allows us to perform magnetic field-induced SIT in the liquid-gated superconducting film. Finite-size scaling analysis indicates that SITs induced both by electric and magnetic field are quantum phase transitions. Moreover, through the comparison of results on two high-Tc cuprates, hole-doped NdBa2Cu3O7-δ (NBCO) and electron-doped PCCO, with different crystal structures, we observed entirely different electrolyte gating mechanisms. We find that field-induced oxygen vacancy formation in CuO chains of NBCO plays the dominant role while it is mainly an electrostatic field effect in the case of PCCO. The possible reason is that NBCO has mobile oxygen in CuO chains while PCCO does not. Our study helps clarify the controversy relating to the mechanism of electrolyte gating, leading to a better understanding of the role of oxygen electro migration which is very material specific.

Strain induced polar metal in $(LaTiO_3)_n/(LaVO_3)_n$ superlattices

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Emergent phenomena in trivalent rare earth oxides heterostructure interfaces have drawn significant attention in the past decade, including metal-to-insulator transitions, 2-dimensional electron gases and multiferroic behaviour. Previous theoretical and experimental work on $LaNiO_3/LaTiO_3$/insulator tri-layered superlattices [1] indicate that inversion symmetry breaking could induce a polar distortion. In this work, we select $(LaTiO_3)_n/(LaVO_3)_n$ superlattices as model system, which have been suggested as a Mott-metal-to-insulator transition system and an unconventional charge transfer system [2]. On $LaGaO_3$ (LGO) twinned single crystal substrate, the superlattice is expected to be in an intermediate state, a so called half metal, which is capable of showing a polar displacement due to c-axis symmetry breaking. These epitaxial samples have been grown on (001) (La,Sr)(Al,Ta)O_3(LSAT), LGO and $SrTiO_3$ (STO), respectively, by pulsed laser deposition (PLD). X-ray diffraction and atomic force microscope methods are used to analyze the crystalline quality and surface topology. We also discuss the resistivity versus temperature as a function of the strain change going from LSAT to STO. We use transmission electron microscopy (TEM) for atomic resolution polarization measurement. X-ray photoelectron spectroscopy or X-ray absorption is used for proving the charge transfer. Based on this analysis we demonstrate that we are able to artificially engineer a polar metal.

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[1] Disa A, Kumah D, Malashevich A, Chen H, Arena D,Specht E, Ismail-Beigi S, Walker F and Ahn C, Phys. Rev. Lett. 114, 026801 (2015)
[2] Weng, Yakui et al. Phys. Rev. B 95, 155117 (2017)

Nonlinear Hall effect originated from the surface of $PdCoO_2$ ultrathin films

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A layered delafossite metal $PdCoO_2$ is one of the most conductive oxides with the bulk conductivity comparable to Au metals.[1,2] Such high conductivity resides in two-dimensional layers of conductive Pd hexagonal sheets and CoO_2 octahedra. This unique anisotropic crystal structure hosts intriguing physical phenomena such as hydrodynamic electron flow induced by the long electron mean free path,[3] anomalous magnetoresistance,[4] and the surface-induced spin-polarized electronic states.[5,6] So far, research on $PdCoO_2$ has been limited in bulk crystals. Recently we have successfully synthesized highly conductive $PdCoO_2$ ultrathin films on Al_2O_3 (0001) substrates by pulsed laser deposition.[7] Thin film growth of $PdCoO_2$ could lead to a new research arena such as the design of heterostructures and devices that exploit the superior transport properties of $PdCoO_2$. Here, we report on the structural characterization and physical properties of $PdCoO_2$ ultrathin films. The sheet conductance of the ultrathin films linearly increases as a function of thickness above the critical thickness about 2 nm that corresponds to the single unit cell of $PdCoO_2$. The room-temperature sheet resistance $R_s < 100$ Ω/sq is achieved for the $d = 4.1$ nm $PdCoO_2$ layers with high optical transparency: the optical transmittance of $PdCoO_2$ thin film $T_{film} > 0.7$ for visible light and $T_{film} > 0.9$ for near infrared light. In addition to the highly conductive features, low-temperature transport measurement shows pronounced non-linearity in the magnetic field dependence of the Hall resistance for thinner samples. We will discuss the origin of the non-linear Hall effect together with the electronic structure studied by angle-resolved photoemission spectroscopy.

[1] A.P. Mackenzie, The properties of ultrapure delafossite metals, Rep. Prog. Phys. 80, 032501 (2017).
[2] R. Daou et al., Unconventional aspects of electronic transport in delafossite oxides, Sci. Technol. Adv. Mater. 18, 919 (2017).
[3] P. J. W. Moll et al., Evidence for hydrodynamic electron flow in PdCoO2, Science 351, 1061 (2016).
[4] H. Takatsu et al., Extremely Large Magnetoresistance in the Nonmagnetic Metal PdCoO2, Phys. Rev. Lett. 111, 056601 (2013).
[5] V. Sunko et al., Maximal Rashba-like spin splitting via kinetic-energy-coupled inversion-symmetry breaking, Nature 541, 492 (2017).
[6] F. Mazzola et al., Itinerant ferromagnetism of the Pd-terminated polar surface of PdCoO2, arXiv:1710.05392.
[7] T. Harada et al., Highly conductive PdCoO2 ultrathin films for transparent electrodes, APL Mater. 6, 046107 (2018).

k-resolved electronic structure of buried oxide and semiconductor interfaces explored by soft-X-ray ARPES

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Pushing ARPES into soft-X-ray energy range (SX-ARPES) enhances its **k**-resolving abilities with larger photoelectron escape depth and chemical specificity achieved with resonant photoexcitation. These virtues allow applications of SX-ARPES to buried interfaces, heterostructures and impurities [1].

Oxide heterostructures. A "drosophila" buried oxide interface is $LaAlO_3/SrTiO_3$ (LAO/STO) embedding mobile 2D electrons. Ti $2p$ resonant SX-ARPES accesses **k**-resolved band structure of the Ti t_{2g} derived charge carriers in the interfacial quantum well (QW). Luttinger count of their Fermi surface identifies phase separation, which is a key element in coexistence of superconductivity with weak ferromagnetism in LAO/STO. The peak-dip-hump spectral lineshape manifests polaronic nature of the interface charge carriers [2,3] where coupling of electrons to the breathing LO3 phonon mode limits their low-temperature mobility, and coupling to the polar TO1 one causes a dramatic mobility drop with temperature. Doping of the LAO/STO interface with oxygen vacancies, affecting electron-phonon coupling, opens ways to tune the interfacial mobility. Further examples include multiferroic $BaTiO_3/La_{1-x}Sr_xMnO_3$ interfaces, etc.

Semiconductor heterostructures. AlGaN/GaN high-electron-mobility transistor (HEMT) heterostructures constitute the basis of the forthcoming 5G telecom technology. SX-ARPES experiment yields Fermi surface, band structure and effective mass of the QW states formed in GaN beneath the AlGaN layer [4]. Their lateral anisotropy, resulting from piezoelectrically active atomic relaxation at the interface, suggests technological measures to increase electron mobility. Photon energy dependence of the ARPES response informs Fourier composition of the QW wavefunctions formed by quantization of the bulk GaN states. Further examples include band offset at the EuO/Si interface, determining its spin injection functionality, local electronic structure of magnetic Mn impurities InMnAs/GaAs quantum dots, superconductor/semiconductor interfaces, etc.

[1] V.N. Strocov et al, Synchr. Rad. News 27, N2 (2014) 31
[2] C. Cancellieri et al, Nature Comm. 7 (2016) 10386
[3] V. N. Strocov et al, in "Spectroscopy of Complex Oxide Interfaces: Photoemission and Related Spectroscopies", eds. C. Cancellieri & V. N. Strocov, Springer, 2018 (arXiv:1612.05791)
[4] L.L. Lev et al, Nature Comm. 9 (2018)

Temperature dependent scanning near-field optical microscopy of $LaAlO_3/SrTiO_3$ interfaces

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The interface between LaAlO3 and SrTiO3 (LAO/STO) hosts a confined two-dimensional conducting electron system (2DES)[1], which exhibits remarkable properties such as superconductivity[2] , spin-orbit coupling, magnetism[3] and gate tunability[4]. Among the experimental techniques applied to this system, optical infrared spectroscopy has been employed to study some important features of the 2DES, in particular, the confinement thickness and the dynamical response of the mobile electrons [5]. However, the spatial mapping capability of the conventional (far-field) infrared spectroscopy is strongly limited by the wavelength.
Here, we employ a cryogenic scanning near-field optical microscopy system (cryo-SNOM) to investigate the LAO/STO interface. The technique allows the mapping of the properties of the 2DES in temperature (5.5 - 300 K) and at different wavelengths (9.3 - 10.6 microns) with an ultra-subwavelength spatial resolution of 10-20 nanometers.
When imaging a sample with conducting and insulating regions defined by optical lithography, we observe that the near-field signal amplitude and, especially, the phase are highly sensitive to the presence of the 2DES. With this technique, we are able to investigate spatial inhomogeneties within the conducting regions, either intrinsic or introduced externally. Importantly, we demonstrate that the SNOM signal is sensitive to electrostatic tuning by a back gate.

[1] Ohtomo A, Hwang H Y. A high-mobility electron gas at the LaAlO3/SrTiO3 heterointerface. Nature, 2004, 427(6973): 423.
[2] Reyren N, Thiel S, Caviglia A D, et al. Superconducting interfaces between insulating oxides. Science, 2007, 317(5842): 1196-1199.
[3] Brinkman A, Huijben M, Van Zalk M, et al. Magnetic effects at the interface between non-magnetic oxides. Nature Materials, 2007, 6(7): 493.
[4] Caviglia A D, Gariglio S, Reyren N, et al. Electric field control of the LaAlO3/SrTiO3 interface ground state. Nature, 2008, 456(7222): 624.
[5] Dubroka A, Rössle M, Kim K W, et al. Dynamical response and confinement of the electrons at the LaAlO3/SrTiO3 interface. Physical Review Letters, 2010, 104(15): 156807.

Scavenging of oxygen vacancies at modulation-doped oxide interfaces: Evidence from oxygen isotope tracing

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The introduction of manganite buffer layers, La7/8Sr1/8MnO3 (LSMO) in particular, at the metallic interface between SrTiO3 (STO) and another band insulator suppresses the carrier density of the interfacial two-dimensional electron gas (2DEG) and improves significantly the electron mobility.[1,2] However, the mechanisms underlying the extreme mobility enhancement remain elusive. Herein, we used 18O isotope exchanged SrTi18O3 as substrates to create 2DEG at room temperature with and without the LSMO buffer layer.[3]By mapping the oxygen profile across the interface between STO18 and disordered LaAlO3 or yttria-stabilized zirconia (YSZ), we provide unambiguous evidence that redox reactions occur at oxide interfaces even grown at room temperature. Moreover, the manganite buffer layer not only suppresses the carrier density but also strongly suppresses the oxygen exchange dynamics of the STO substrate, which likely prevents the reduction of STO during the formation of the 2DEG. The underlying mechanism on the enhanced electron mobility at buffered oxide interfaces is also discussed.

[1] Y. Z. Chen et al. Nature Mater. 14 (8), 801 (2015)
[2] Y. Z. Chen, R. J. Green, R. Sutarto, F. He, S. Linderoth, G. A. Sawatzky, and N. Pryds. Nano Lett. 17, 7062-7066 (2017)
[3] Y. Z. Chen, M. Döbeli, E. Pomjakushina, Y. L. Gan, N. Pryds, and T. Lippert. Phys. Rev. Materials 1, 052002(R) (2017)

Probing the superconducting state of $SrTiO_3/LaAlO_3$ by superconducting coplanar waveguide resonators

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Since its discovery, the two-dimensional electron gas found at the interface between bulk $SrTiO_3$ (STO) and $LaAlO_3$ (LAO) thin films has been intensely studied, with a focus on two-dimensional superconductivity and its interplay with spin-orbit coupling and magnetic properties.
Coplanar waveguide resonators are a very useful tool to investigate two-dimensional superconductivity. Their low ohmic losses make them very sensitive to excitations in circuit and materials. This makes CPW's interesting candidate as a sensitive probe of electronic properties of materials. In this work, we study the superconducting state of (100) STO/LAO interfaces probed by superconducting coplanar waveguide resonators. These devices provide direct access to the superfluid density in macroscopic regions of the LAO/STO interfaces. We characterized the CPW spectral response as a function of temperature, back-gate voltage, and power of the RF field. We find a non-monotonic dependence of the superfluid density on the applied back-gate voltage. We will discuss the gate tuning of Cooper pair density in the underdoped and overdoped regions of the phase diagram, highlighting key differences. We will also emphasize the broad applicability of coplanar waveguide resonators in the study of oxide interface physics.

Metallic Conduction and Ferromagnetism in MAl2O4/SrTiO3 Spinel/Perovskite Heterostructures (M = Fe, Co, Ni)

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Besides perovskite-type oxide interfaces [1], a high mobility quasi-two-dimensional electron gas (q-2DEG) can also be formed at the spinel/perovskite heterointerface of γ-Al2O3 and SrTiO3 (STO)[2]. In this work, we fabricated the epitaxial heterostructure with Al-based magnetic spinel oxide MAl2O4 (M = Ni, Co and Fe) and STO. Remarkably, the NiAl2O4/STO and CoAl2O4/STO heterointerfaces are highly metallic and ferromagnetic. The electron mobility is as high as 3 × 104 cm2V-1s-1 and anomalous Hall effect (AHE) persists up to 30 K, much higher than 5 K as for the γ-Al2O3/STO interface. Compared to that of γ-Al2O3/STO, moreover, the anomalous Hall resistance exhibits an opposite sign and is enhanced by more than three times. In contrast, the FeAl2O4/STO is insulating. The AHE in γ-Al2O3/STO could be due to the presence of oxygen-vacancy-related magnetism, while the AHE in NiAl2O4/STO and CoAl2O4/STO likely comes from magnetic impurity effect due to the interdiffusion of magnetic ions from capping layers into the STO surface.

[1] A. Ohtomo and H. Y. Hwang, Nature 427, 423 (2004)
[2] Y. Z. Chen, N. Bovet, F. Trier, D. V. Christensen, F. M. Qu, N. H. Andersen, T. Kasama, W. Zhang, R. Giraud, J. Dufouleur, T. S. Jespersen, J. R. Sun, A. Smith, J. Nygard, L. Lu, B. Buchner, B. G. Shen, S. Linderoth, and N. Pryds, Nat. Commun. 4, 1371 (2013)

Charge- versus orbital-order in e_g^1 perovskites

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Rare-earth nickelates ($RNiO_3$), rare-earth manganites ($RMnO_3$), and alkaline-earth ferrites ($AFeO_3$), are perovskites sharing the same formal single-electron occupation of the transition metal e_g orbitals. At high temperatures, these oxides show a metallic behavior. On cooling, they typically exhibit a metal to insulator transition (MIT) but through different mechanisms. On the one hand, $RMnO_3$ perovskites show an orbital-order type MIT and Jahn-Teller distortion of the oxygen octahedra while $ReNiO_3$ and $CaFeO_3$ exhibit a charge-order type MIT and breathing distortion of the oxygen octahedra. We show that the tendency to either charge- or orbital-order type transition is not an exclusive intrinsic property of each family of compound but has to be thought as tunable. From ab-initio calculations, we first clarify the structurally triggered mechanism at the origin of the charge-order type MIT in nickelates [1] and ferrites [2]. We then demonstrate that an alternative orbital-order MIT can be engineered under tensile epitaxial strain in these compounds [2]. Finally, we propose different possibilities in the e_g^1 family to create new multiferroic materials, highlighting how fundamental understanding of the interplay between magnetic, electronic properties and structural distortions can lead to new design paths toward exciting materials.

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[1] *Structurally triggered metal-insulator transition in rare-earth nickelates.* A. Mercy, J. Bieder, J. Iniguez and Ph. Ghosez, Nature Communications **8**, 1677 (2017).
[2] *From charge- to orbital-order type metal-insulator transition in alkaline-earth ferrites.* Y. Zhang, M. M. Schmitt, A. Mercy, J. Wang and Ph. Ghosez, unpublished.

The coupled structural and electronic metal-insulator transition in rare earth nickelates from DFT+DMFT

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Rare earth nickelates, $R\mathrm{NiO_3}$, exhibit a metal-insulator transition that is accompanied by a structural distortion that breaks the symmetry between formerly equivalent Ni sites. Here we show, using density functional theory combined with dynamical mean-field theory (DFT+DMFT), that this transition is related to an electronic instability towards a spontaneous "charge diproportionation" of the Ni cations, which couples strongly to a breathing mode distortion of the octahedral network. Using screened interaction parameters calculated within the constrained random phase approximation, our DFT+DMFT total energy calculations predict amplitudes for the distortion that are in excellent agreement with available experimental data. Furthermore, our results also indicate that for both $\mathrm{NdNiO_3}$ and $\mathrm{PrNiO_3}$ the simultaneous presence of antiferromagnetic order is required to stabilize the lattice distortion, in agreement with other recent reports [1,2]. Our work also highlights the predictive capabilities of the DFT+DMFT approach for coupled electronic and structural properties in correlated electron materials. [Parts of this work have been performed in collaboration with Oleg Peil (Materials Center Leoben), Antoine Georges (College de France), Peitao Liu, and Cesere Franchini (both University of Vienna).]

[1] K. Haule and G. L. Pascut, Scientific Reports 7, 10375 (2017).
[2] A. Mercy et al., Nature Communications 8, 1677 (2017).

First-principles study of ferroelectricity, antiferroelectricity and polarons in WO_3

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Tungsten trioxide WO_3 is a very unique transition-metal oxide because it has a simple A-site vacant ABO_3 perovskite structure with numerous properties such as electrochromicity, thermochromicity, piezoelectricity, superconductivity, etc. This makes WO_3 of high interest in diverse technological applications relying on these properties such as smart windows, sensors, displays, photocorosion, solar cells, etc. However, despite the intensive studies made on WO_3, a microscopic understanding of the underneath mechanisms responsible for its exceptional responses is still lacking. Here we pave the road on this shortage by investigating WO_3 properties from first-principles density functional theory calculations using hybrid functionals. In a first step our structural analysis shows that the ground state of WO_3 is actually antiferroelectric with metastable ferroelectric phases close in energy. In a second step we report an unprecedented first-principles electronic and structural characterization of isolated self-trapped polarons and bi-polarons in crystalline WO_3. Our results are of high importance to understand the properties of off-stoichiometric WO_{3-x}, which is at the source of all of the chromic and superconducting responses. Going beyond we will discuss its potential new properties related to the large spin orbit coupling present in W atom such as Rashba spin splitting.

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Engineering large and reversible Rashba spin splitting in ferroelectric perovskite oxides and related compounds

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Ferroelectric Rashba semiconductors (FERSC), in which Rashba spin-splitting can be controlled and reversed by an electric field, have recently emerged as a very exciting new class of functional materials. However, full exploitation of the concept is still hampered by the lack of known robust ferroelectric compounds showing large Rashba spin splitting. Here, we rationalize the search of efficient FERSC within the family of perovskite oxides relying on first-principles calculations. We first highlight that the coexistence of large spontaneous polarisation and spin-orbit coupling is not sufficient to have good FERSC properties and we establish why simple ferroelectric oxide perovskites with transition metal at the B-site are typically not suitable candidates. Then, we show how this intrinsic limitation can be by-passed through interface engineering of the electronic band structure in layered perovskites and identify the ferroelectric Bi_2WO_6 Aurivillius phase as a promising FERSC compound. The role of distinct atomic distortions on the Rashba spin splitting is discussed. We further show that Bi_2WO_6 preserves its ferroelectric properties over substantial n-doping. This last feature also makes it attractive for other applications, which will be briefly discussed.

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First-principles study of $SrTiO_3(001)/LaAlO_3/SrTiO_3$ heterostructures

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The origin of the 2-dimensional electron liquid (2DEL) appearing at the interface of band insulators $SrTiO_3$ (STO) and $LaAlO_3$ (LAO) has been rationalized in the framework of a polar catastrophe, related to the critical thickness of the polar LAO overlayer needed for the appearance of the 2DEL: built-in field divergence is avoided either through an electronic reconstruction or a stabilization mechanism of donor defects (such as oxygen vacancies) at the LAO surface, both providing electrons, doping the interface. It has been shown experimentally that it is possible to observe conduction below the critical thickness, down to 1 monolayer of LAO, by capping the LAO layer with STO [1, 2], questioning the validity of these two polarity-driven mechanisms. Here, we investigate step-by-step these mechanisms from hybrid functional-based DFT calculations on $STO(001)/LAO_m/STO_n$ heterostructures. We then discuss the relevance of the two pictures in relation with experimental observations.

[1] M. Huijben et. al., Nature Materials 5, 556 (2006)
[2] R. Pentcheva et. al., Phys. Rev. Lett. 104, 166804 (2010)

BoSS your oxide

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The electronic structure of transition metal oxides is often affected significantly by strong and localized electron-electron interactions. Examples include renormalization of the mass and spectral weight of low energy quasiparticles and the formation of Hubbard bands: these dynamical effects can not be described by band theory approaches (e.g., DFT, DFT+U or hybrid methods). Slave-boson approaches represent computationally efficient electronic structure methods that can include such effects explicitly. We summarize our recent slave boson methodology [1,2], apply it to oxides and compare to experimental and dynamical mean field theory (DMFT) results, and introduce BoSS (Boson Slave Solver) — an open source software release implementing this approach.

[1] Georgescu and Ismail-Beigi, PRB 92, 235117 (2015).
[2] Georgescu and Ismail-Beigi, PRB 96, 165135 (2017).

Toward a unified view on the metal-insulator transition in nickelates

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The mechanism of metal-insulator transition in nickelate is a long-standing puzzle. Several models have been proposed from different approaches, each being successful in its own perspective but sometimes conflicts with others. Here we parameterize an effective Hamiltonian on both the lattice distortion and the electronic structure of nickelates from DFT simulations. By analyzing these effective hamiltonians, we scrutinize the mechanisms of the MIT in nickelates by taking into account the couplings among electron, lattice, and spin. Meanwhile we compare the results with existing models and try to understand them from a unified view.

Ferromagnetic insulating perovskite for nonvolatile memory device and anisotropic sensor

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In the past decade, great scientific efforts have been dedicated to the development of much more efficient technology for storing, reading and securing information. Devices based on spin manipulation have conferred important advantages in front of conventional semiconductor devices as non-volatility, low dissipation, faster processing speed, etc. Hence, spin-polarized devices such as magnetic tunnel junctions (MTJ) are the main building blocks of spin-based electronic components such as MRAM. In here, we investigate the possibility of using a ferromagnetic insulating material in a MTJ device. The device consists of $Pt/La_2Co_{0.8}Mn_{1.2}O_6/Nb{:}SrTiO_3$ heterostructure where the barrier is the only magnetic material. Uniquely, $La_2Co_{0.8}Mn_{1.2}O_6$ ($T_C \approx 230\,K$) thin films present strong perpendicular magnetic anisotropy (PMA) whose origin lies in the large spin-orbit interaction of Co^{2+} which is additionally tuned by the epitaxial strain [1,2]. We prove sensor and memory functionalities based on Tunneling Anisotropic Magnetoresistance (TAMR). Besides an estimated spin-filtering efficiency of near 100%, PMA induces in these structures TAMR values up to 30%. Moreover, the strong anisotropy of magneto-transport properties makes the device to present two different zero-field resistance states [3]. Therefore, we introduced essentially a proof of concept of a spintronic device that represents an alternative of easier technological implementation, avoiding the need of two magnetically decoupled ferromagnetic electrodes and coherent tunneling.

[1] Galceran, R. et al. Phys. Rev. B **93**, 144417 (2016).
[2] López-Mir, L. et al. Phys. Rev. B **95**, 224434 (2017).
[3] López-Mir, L. et al. Sci. Reports **8**, 861 (2018).

Mapping Electrochemical Activity at the Nanoscale for Enhanced Solid-State Battery Electrodes

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Solid-state microbatteries can facilitate miniaturization, create more flexibility for the design of stand-alone microelectronic devices and enhance their applicability. However, the successful application of all-solid-state microbatteries depends strongly on the enhancement of energy density and lifetime. The cycle-life and lifetime are dependent on the nature of the interfaces between the electrodes and electrolyte, whereas safety is a function of the stability of the electrode materials and interfaces. Therefore, perfect control on the interfacial properties between the electrodes and electrolyte is needed but remains a great challenge.

Various oxide materials are known as promising cathode materials as they provide good thermochemical stability, high energy density and high voltage. $LiMn_2O_4$ is a suitable candidate for the cathode electrode. This spinel compound offers favorable safety and intrinsic rate capability, which arise from the chemically stable Mn^{3+}/Mn^{4+} couple and a 3D framework for facile Li^+ mobility [1,2]. Common bulk studies on battery materials investigate polycrystalline films and, therefore, do not enable detailed characterization of the ionic and electrical conductivity along specific crystalline orientations.

SPM techniques allow us to measure the electrochemistry taking place on the nanoscale, which can be used to elucidate structure/function relationships in battery materials with exceptional resolution. To achieve insight into the non-uniform distribution of lithium activity at the cathode-electrolyte interface, First Order Reversal Curve current-voltage (FORC-IV) analysis [3,4] is applied. This technique enables the probing of nanoscale electrochemistry due to the capability to measure local ionic currents. In FORC-IV measurements, current through the sample is measured with an AFM probe in contact mode as a function of the bias waveform, a triangular wave with increasing amplitude, allowing the measurement of a variety of electrochemical processes. Depending on the rate and reversibility of these processes, this will result in hysteretic I-V curves, proportional to the voltage-activated electrochemical processes and transport at a given spot.

Here, we have studied the local lithium diffusion in $LiMn_2O_4$ thin films, epitaxially grown by Pulsed Laser Deposition on single crystalline Nb-doped $SrTiO_3$ substrates. Control over the specific crystal orientation of the full thin film enables detailed analysis of the lithium diffusion along specific crystal planes (001, 110 and 111). By changing the crystal orientation of the underlying single crystalline substrate, we can control the specific orientation of the $LiMn_2O_4$ thin film and, therefore, the cathode surface towards the electrolyte. The FORC results expose the electrochemical activity for different crystal facets indicating the topography dependent lithium diffusion. These results provide better understanding of the importance of the specific crystal facet in contact with the adjacent electrolyte to enable enhanced engineering of the interfacial properties.

[1] M. E. Spahr , P. Novák , Adv. Mater. 10 (1998) 725.
[2] M.M. Thackeray, Progr. Solid State Chem. 25 (1997) 1.
[3] E. Strelcov, et al., Nano Lett. 13 (2013) 3455-3462.
[4] Y-H Hsieh, et al., ACS Nano 7(10) (2013) 8627-8633.

Hydrogen plasma induced Mott-insulating and transparent-conducting states in epitaxial $Ba_{0.5}Sr_{0.5}TiO_3$ thin-films

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Transparent conducting oxides (TCO's) are one of the key materials for optoelectronic device applications such as display panels and solar cells[1]. Widely used TCO's such as indium-doped tin oxide (ITO) exhibit high electrical conductivity (> 1 kΩ^{-1}cm^{-1}) and good optical transparency ($> 80\%$)[2]. Recently, complex oxide thin-films such as vanadates[3] have been suggested as new TCO's by utilizing the large effective mass of strongly-correlated electrons. Such a large effective mass of electrons can help lower plasma frequencies below 1.5 eV even with relatively large carrier concentrations ($n = 10^{22}$ cm^{-3}). However, conventional chemical doping on complex oxides often results in unwanted impurity bands which deteriorate their optical transparency[4]. Thus, we ask, "Can we introduce enough mobile strongly-correlated electrons into wide-gap complex oxides ($E_g > 3$ eV) without forming light-absorbing impurity bands?"

In this presentation, we report that epitaxial $Ba_{0.5}Sr_{0.5}TiO_3$ (BST) thin-films exhibit phase transitions from a wide-gap insulator to a Mott insulator and eventually to a transparent conductor via hydrogen-plasma exposure (HPE). BST thin-films are well-known robust insulators; no chemical doping methods, including oxygen vacancies[5], can generate conducting carriers effectively. Our pulsed laser deposited BST thin films on $GdScO_3$ substrates show optically transparent and insulating properties. After about 2 minutes of HPE, the samples exhibit an intriguing absorption band at infrared energies with a small optical gap around 0.2 eV, which is similar to Mott insulators such as $LaTiO_3$ and $YTiO_3$[6]. Further HPE up to about 5 minutes makes the samples exhibit a Drude response below 1.5 eV in the optical spectra with a dc-conductivity of 413 Ω^{-1}cm^{-1}, which implies that a correlated metallic state is created. The optical transparency of the BST thin films after the 5 minutes of HPE remains the same as unexposed samples in the visible region. We will discuss how HPE can open a new way for realizing insulator-to-metal transitions by introducing strongly-correlated electrons into complex oxide thin films.

[1] S. H. Keshmiri *et al.* Thin Solid Films **413**, 167 (2002).
[2] T. Minami Semiconductor Science and Technology **20**, S35 (2005).
[3] L. Zhang *et al.* Nat. Mat. **15**, 204 (2016).
[4] C. Lee, J. Destry, & J. L. Brebner Phys. Rev. B **11**, 2299 (1975).
[5] X. Liang *et al.* Journ. Of Amer. Ceram. Soc. **87**, 2218 (2004).
[6] T.-h. Arima & Y. Tokura J. Phys. Soc. Jpn. **64**, 2488 (1995).

Atomically interface engineered micrometer-thick oxide electrodes for thin dielectrics tunable at ion battery voltage

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The exemplary story of the CMOS microelectronic technology shows that modern electronic devices require various functional layers of a thickness up to a few micrometers, combined with atomically engineered interfaces controlled at the unit cell level. Considering realization of oxide electronic devices for high-frequency applications such as low-loss tunable filters and antennas, the desired thickness of the conducting oxide electrode is determined by the electromagnetic skin depth which increases with resistivity of the electrode material and has a value of the order of several micrometers in the frequency range of a few GHz. Among the known conductive oxide perovskites, the smallest skin depth is achieved in single crystal of $SrMoO_3$ due to its low resistivity of 5 $\mu\Omega$cm at room-temperature outperforming even Pt (10.6 $\mu\Omega$cm), thus, making $SrMoO_3$ a prominent conducting electrode material for high-frequency microelectronic devices [1-5].

Here we present an $Au/Pt/Ba_{0.5}Sr_{0.5}TiO_3/SrTiO_3/SrMoO_3$ parallel-plate varactor with the heteroepitaxial perovskite oxide stack comprised of a 5 μm thick conducting bottom electrode of $SrMoO_3$, a 50 nm thin isostructural tunable dielectric layer of $Ba_{0.5}Sr_{0.5}TiO_3$, and a 10 unit-cells-thick $SrTiO_3$ interlayer used to separate these functional layers with extremely contradicting thermodynamic phase diagrams [6]. The stack was grown layer-by-layer using pulsed laser deposition on $GdScO_3$ substrates with all involved lattice mismatches below 0.5%. The difficult-to-access epitaxial layer-by-layer thick-film growth makes use of the extraordinary ability of $SrMoO_3$ to accommodate strain by adjusting its lattice constant with small shifts in the cation ratio, tuned by pulsed laser deposition parameters. X-ray and reflective high-energy electron diffraction measurements and high-resolution transmission electron microscopy revealed perfect perovskite structure throughout the complete thickness of the oxide stack with atomically flat interfaces between the layers.

The used low-resistive $SrMoO_3$ thin-film oxide electrode leads to low losses and high quality factor Q of the varactors. The layer-by-layer grown epitaxial $Ba_{0.5}Sr_{0.5}TiO_3$ results an unprecedentedly high capacitance (C) tunability of $n(3.7\text{ V}) = C(0)/C(3.7\text{ V}) = 3.1$ at the Li-ion battery voltage level of 3.7 V. Thus, the obtained high aggregate performance of the varactors expressed in the high values of the "standard" commutation quality factor CQF (1GHz) ≈ 3700 and the more relevant voltage performance factor $\text{VPF}(3.7\,\text{V}, 1\,\text{GHz}) = n(3.7\text{ V}) \cdot Q(0\,\text{V}, 1\,\text{GHz})/3.7\,\text{V} \approx 65$ stands out in the gigahertz frequency range of interest and is comparable.

[1] I. Nagai et al. Appl. Phys. Lett. 87, 024105 (2005).
[2] A. Radetinac et al. Appl. Phys. Express 3, 073003 (2010).
[3] A. Radetinac et al. Appl. Phys. Lett. 105, 114108 (2014).
[4] L. Alff et al., J. Phys. D: Appl. Phys. 47, 034012 (2014).
[5] A. Radetinac et al. J. Appl. Phys. 119, 055302 (2016).
[6] A. Radetinac et al. J. Cryst. Growth. 463, 134 (2017).

Generation and detection of surface acoustic waves on strain-induced piezoelectric $SrTiO_3$

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$SrTiO_3$ does not show piezoelectricity because of its centrosymmetric crystal structure. Strain, however, can alter the crystal structure and induce piezoelectricity in $SrTiO_3$. Strain can be obtained in three different ways: (1) at low temperature, (2) by applying a dc electric field, or (3) by bi-layer formation with a lattice-mismatched film deposited on top [1-3]. Here, we focus on contributions of the first two effects by generation and detection of surface acoustic waves (SAWs), which requires a piezoelectric substrate or thin film. In our experiments, SAWs were generated by applying an RF-signal to metallic inter-digitated transducers (IDTs) directly on top of a $SrTiO_3$ substrate in delay-line configuration. Various types of transducers were investigated, and the effect of the number of IDT fingers and the distance between the generating IDT and detecting IDT was analyzed. Our results imply that, SAWs is generated on strain-induced piezoelectric $SrTiO_3$ and the transmission of SAWs is enhanced as the temperature is lowered.

[1] Science, 276, 392 (1997)
[2] Appl. Phys. Lett. 105, 062901 (2014)
[3] Journal of Applied Physics 102, 044119 (2007)

Steep-slope NbO_2-based threshold switch enabled by pulsed-laser-induced phase transformation

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The correlated oxides, including NbO_2, show promising potential for threshold switching device in that it prevents sneak current in 3D cross-point array architecture and overcomes a limitation of subthreshold swing (SS < 60mV/dec) owing to high theoretical I_{on}/I_{off} ratio ($\leq 10^7$), fast switching speed ($\geq$22 ns) and thermal stability at device-working temperature[1−2]. However, to realize voltage-induced insulator-to-metal transition with a NbO_2, high-temperature processes, such as growth or post-annealing at high temperature, were required for crystallization (>573K) to observe voltage-induced insulator-to-metal transition (IMT), this high-temperature processing needs to be avoided due to degradation by unwanted layers and high energy consumption[3]. Moreover, due to the multivalency of Nb cation, there was very limited oxygen partial pressure (pO_2) window to stabilized Nb^{4+} valence states during the NbO_2 film growth[3]. In contrast, pulsed laser annealing, which generates temperature field at confined area, is powerful tool for rapid crystal growth and a reduction reaction is also possible by changing process environment.

In this research, we report new strategy for fabricating high performance threshold switch with correlated oxides NbO_2 using pulsed laser annealing, showing steep voltage-induced insulator-to-metal transition. As the number of pulses and process environment were accurately controlled during laser annealing, the as-grown Nb_2O_5 films were transformed into NbO_2 by forming stable Nb^{4+} valence states. The fabricated selector device using laser-annealed NbO_2 films shows low off-current ($\sim$665 nA) and high I_{on}/I_{off} ratio (>230) without high temperature process. A comprehensive study with transmission electron microscopy and synchrotron X-ray photoemission spectroscopy reveals that the crystallization combined with oxygen loss stimulates the formation of stable NbO_2 crystallites in the films during pulsed laser annealing. Our approach provides novel solution for facile fabrication of high-performance correlated oxide-based selector device with steep transition.

[1] You, Z. & Ramanathan, S. Mott Memory and Neuromorphic Devices. Proceedings of the IEEE 103, 1289-1310 (2015).

[2] Shukla, N. et al. A steep-slope transistor based on abrupt electronic phase transition. Nat Commun. 6, 7812 (2015).

[3] Kang, M. & Son, J. Off-state current reduction in NbO_2-based selector device by using TiO_2 tunneling barrier as an oxygen scavenger. Applied Physics Letters 109 (2016).

Polycrystalline ceramics: a new generation of substrates using combinatorial epitaxy

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Complex oxide materials have an exceptionally broad range of versatile functionalities such as High Tc superconductivity, colossal magnetoresistance or multiferroic; often dependent on crystallographic orientation and controllable by external stimuli (electric/magnetic fields, light, stress,...) Furthermore, improvement of deposition technics let us control the This area of research was boosted by numerous improvements like the possibility to the growth of well-defined heterostructures as epitaxial thin films with atomically smooth surfaces or interfaces. When used appropriately, novel properties emerge or become significantly different from the bulk compound. Usually, thin films are deposited on a monocrystalline substrate (i.e. presenting a unique out of plan orientation) and generally, commercial substrates are often limited to low index orientation as (100), (110) or (111).
The Combinatorial Substrate Epitaxy (CSE) is a new approach, where the film is deposited on a polycrystalline substrate. The surface presents all the possible orientations, and each ten of micrometer-size grain can be viewed as a single crystal. The sample is a multi-oriented film prepared in a single experiment, opening the route to a complete study by Electron BackScatering Diffraction (EBSD) of the orientation relationship between the films and the substrate as we can control a grain-over-grain growth [1-5]. CSE is an interesting option to enlarge the spectra of physical properties in a single film deposited on a low-cost substrate.

Here, we present our methodology of synthesis and characterization of polycrystalline substrates, as well as new results regarding $La_{0.7}Sr_{0.3}MnO_3$ thin films deposited on $SrTiO_3$ and $LaAlO_3$ polycrystalline substrate. Particularly, we observe the same saturation magnetization for both configurations compare to single crystal, and, we will show new magneto-transport properties induced by the CSE approach.

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[1] Lacotte et al., J. Appl. Phys. 116, 245303 (2014)
[2] Pravarthana et al., Appl. Phys. Lett. 104, 082914 (2014)
[3] Lacotte et al., J. Appl. Phys. 118, 045306 (2015)
[4] Woo et al., Scientific Reports, 5 : 8822 (2015)
[5] Santosh et al., J.Phys. D : Appl. Phys. 50 (2017) 235301

Real-time observation of reversible topotactic phase transition in epitaxial $SrFeO_x$ thin films.

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Spontaneous oxygen vacancy ordering in transition metal oxides provides an interesting platform for studying thermodynamic stability of a crystal lattice. Technologically, different materials properties can be tuned by controlling the oxygen vacancies, which are relevant for various energy and environmental applications exploiting the redox reactions, such as solidoxide fuel cells, gas sensors and rechargeable batteries. In this context strontium ferrite ($SrFeO_x$) is a potential material as it can adopt various oxidation states due to the multivalent nature of Fe and shows intriguing spontaneous oxygen vacancy ordering.

In this work, we examined the topotactic transformation of $SrFeO_x$ epitaxial thin films using real-time spectroscopic ellipsometry. Two structurally distinctive phases, i.e., perovskite ($SrFeO_3$) and brownmillerite ($SrFeO_{2.5}$), could be reversibly obtained by changing the oxygen partial pressure and temperature of the sample. The x-dependent change in the dielectric function clearly indicates that the rapid topotactic phase transformation at relatively low temperature accompanies a drastic change in the crystallographic and electronic structures. Our results provide an insight into the phase stability and reversibility of technologically important $SrFeO_x$.

Atomic control of disorder in PZT and epitaxial integration on GaN for high-power devices

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Due to its physical properties gallium-nitride (GaN) is gaining a lot of attention as an emerging semiconductor material in the field of high-power and high-frequency electronics applications. Therefore, the improvement in the performance and/or perhaps even extension in functionality of GaN based devices would be highly desirable. The integration of ferroelectric materials such as lead-zirconate-titanate ($PbZr_xTi_{1-x}O_3$, PZT) with GaN has a strong potential to offer such an improvement. However, the large lattice mismatch (9%) between PZT and GaN makes the epitaxial growth of on GaN a formidable challenge. Our starting point is based on previous work, which introduced a novel strain relaxation mechanism observed when MgO is used as a buffer layer, with thicknesses down to a single unit cell, inducing epitaxial growth of high crystallinity (PZT) thin films [1].
Here, we will discuss the large dielectric constant of PZT, of technological interest in transistors, and our attempt to control it by tailoring PZT structure at the atomic scale. More precisely, the amount of disorder in the system is tuned by growing epitaxial layers of PZTwith alternating tetragonal and rhombohedral order, inducing large strain and interface effects in the superlattices. Among its technological interest, this work sheds light on fundamental properties of disorder in systems showing a morphotropic phase boundary.

[1] L. Li et al., *Epitaxial Stress-Free Growth of High Crystallinity Ferroelectric PbZr 0.52 Ti 0.48 O 3 on GaN/AlGaN/Si(111) Substrate*, Adv. Mater. Interfaces **5**, 1700921 (2018)

Complex oxidation behavior of $W_xTi_{1-x}O_y$ alloys

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TiO_2 and WO_3 are two of the most important earth-abundant materials for electronic and energy applications. Particularly for smart windows, WO_3 is one of best performing materials to date. It has been demonstrated that alloying WO_3 with TiO_2 can improve both performance and stability of such electrochromic devices[1]. While the oxidation of both W and Ti has been discussed in literature, only few works exist on the oxidation of W-Ti alloys.

In this work we present an in-depth study of the oxidation behavior in W-Ti alloys using different synthesis routes. Solid solution alloy precursors were deposited using combinatorial sputtering and subsequently oxidized using either thermal oxidation or potentiostatic anodization, which correspond to near-equilibrium and off-equilibrium growth methods, respectively. The oxide formation during thermal oxidation and the thermal stability of the anodic oxide alloys were monitored using real time synchrotron XRD. For both oxidation methods a Ti-enrichment in the surface region of the grown $W_xTi_{1-x}O_y$ layer is observed, which strongly depends on the oxidation conditions and precursor composition. As evidenced by XPS mapping and TEM, a thin TiO_2 overlayer on top of the $W_xTi_{1-x}O_y$ film can be achieved, resulting in an increased stability in reactive environments. In addition, the optoelectronic properties of the oxide are reported, providing insights into the synthesis-property relationship of $W_xTi_{1-x}O_y$.

[1] Sol.Energ.Mat.Sol.Cells 125,184-189,2014

Electronic transport in (110) SrIrO3 heterostructures

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SrIrO3 (SIO) films epitaxially grown on orthorhombic (110) GdScO3 (GSO) and DyScO3 (DSO) are found to display bulk-like orthorhombic structure with space group Pbnm. Film deposition on cubic (001) SrTiO3 or (LaAlO3)0.3(Sr2AlTaO6)0.35 (LSAT) results in a twinned growth of SIO. Resistance measurements on the SIO films reveal only weak temperature dependence, where R increases with decreasing T, indicating the proximity to a metal-to-insulator transition. Hall measurements show dominant electron-like transport throughout the temperature range from 2 K to 300 K. Interestingly, the film resistances for the two orthogonal directions along the substrate edges of GSO and DSO are not the same and differ by up to 25% indicating pronounced anisotropic behavior with a specific T-dependence. The measurements indicate that structural changes of the substrate material are likely responsible for the observed anisotropic electronic transport. The substrate-induced effects are likely related to constraints with respect to IrO6 octahedral rotations. The strong sensitivity of the electronic transport in SIO films to substrate-induced structural changes may be explained in terms of the narrow electron-like bands in SIO caused by spin-orbit-coupling and orthorhombic distortion.

UV radiation enhanced oxygen vacancy formation caused by the PLD plasma plume

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Pulsed Laser Deposition is a commonly used non-equilibrium physical deposition technique for the growth of complex oxide thin films. A wide range of parameters is known to influence the properties of the used samples and thin films, especially the oxygen-vacancy concentration. One parameter has up to this point been neglected due to the challenges of separating its influence from the influence of the impinging species during growth: the UV-radiation of the plasma plume. We here present experiments enabled by a specially designed holder to allow a separation of these two influences. The influence of the UV-irradiation during pulsed laser deposition on the formation of oxygen-vacancies is investigated for the perovskite model material $SrTiO_3$. The carrier concentration of UV-irradiated samples is nearly constant with depth and time. By contrast samples not exposed to the radiation of the plume show a depth dependence and a decrease in concentration over time. We reveal an increase in Ti-vacancy-oxygen-vacancy-complexes for UV irradiated samples, consistent with the different carrier concentrations. We find a UV enhanced oxygen-vacancy incorporation rate as responsible mechanism. We provide a complete picture of another influence parameter to be considered during pulsed laser depositions and unravel the mechanism behind persistent-photo-conductivity in $SrTiO_3$.

Single-crystal Strontium Aluminate thin films by pulsed laser deposition

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$SrAl_2O_4$ co-doped with Eu and Dy is one of the most studied luminescent phosphors with strong and long persistant emission. The long afterglow effect is usually explained by electron trapping at defect center with energy states below the conduction band, such as oxygen vacancy or controlled defects related to Dy dopant.[1-3] The exact trapping mechanism is however still under debate due to the complexity of conventional powder system, such as the interferences from crystallinity, grain size, grain boundary and so on. High quality single-crystal could offer the possibility to investigate the effect of controlled defects on the trapping mechanism. In this study, epitaxial growth of single-crystal $SrAl_2O_4$ film on sapphire substrate was successfully achieved by means of pulsed laser deposition. Film growth was monitored *in-situ* by reflection high-energy electron diffraction (RHEED). The obtained films were characterized by XRD and TEM, based on which the epitaxial orientation relation between film and substrate was determined.

[1] T. Matsuzawa, Y. Aoki, N. Takeuchi and Y. Murayama, Journal of the Electrochemical Society 143 (1996) 2670-2673.
[2] P. Dorenbosz, Journal of the Electrochemical Society 152 (2005) H107-H110.
[3] Frédéric Clabau, Xavier Rocquefelte, Stéphane Jobic, Philippe Deniard, Myung-Hwan Whangbo, Alain Garcia, Thierry Le Mercier, Solid State Sciences 9 (2007) 608-612.

Effect of $Ba_xSr_{1-x}HfO_3$ buffer layer on La-doped $BaSnO_3$

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La-doped BaSnO3(BLSO) is a wide bandgap semiconducting perovskiteoxide with highelectron mobilityand excellent oxygen stability at room temperature [1]. In recent reports on the excellent carrier modulation of BLSO channel by field effect on perovskite SrTiO3 (STO) [2] and non-perovskite MgO [3], we found an optimized un-doped BaSnO3 (BSO) buffer layer thickness to be around 150 nm. However, BSO shows persistent and large photoconductivity under the light with wavelength smaller than 400 nm [4]. To prevent the change of channel conductance by such photoconductivity of the BSO buffer layer, we fabricated an atomically-mixed BaxSr1-xHfO3 (BSHO, with x varying from 0 to 0.9) buffer layer. Both BaHfO3 (BHO) and SrHfO3 (SHO) have wider bandgaps than BSO (5.8 eV and 6.1 eV respectively) and show no measurable photoconductivity. We reduced BSHO lattice mismatch with BLSO by finding a suitable ratio of BHO to SHO. We will report on the field effect transistor performances with BSHO as a buffer layer and BLSOas the channel layer and compare them with those of previous samples using a BSO buffer layer.

[1] H. J. Kim, U. Kim et al., Appl. Phys. Express 5, 061102 (2012).
[2] U. Kim et al., APL Mat. 4, 071102 (2016).
[3] Juyeon Shin et al., Appl. Phys. Lett. 109, 262102 (2016).
[4] Jisung Park et al., Appl. Phys. Lett. 108, 092106 (2016)

Preparation of atomically flat, single terminated $LaAlO_3$ (001) substrate surfaces through thermal annealing and deionized water leaching

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Atomically flat, chemically uniform oxide substrate surface is a prerequisite for constructing abrupt interfaces and investigating emergent phenomena at oxide interfaces. [1, 2] Despite the vast use of $LaAlO_3$ (001) substrate, its role as a template for the interface physics is not many. It is probably due to a lack of well-established recipes for atomically flat, single terminated $LaAlO_3$ (001) substrate surfaces. We found that the surface reconstruction of $LaAlO_3$ (001) limits the simultaneous achievement of atomic flatness and single termination. [3] To overcome it, we exploit the water solubility of the annealed $LaAlO_3$ (001) surface. Using atomic force microscopy, we investigate and visualize the detailed dissolution procedure of $LaAlO_3$ (001) surface layers during water leaching. After an appropriate amount of water leaching step, we achieve atomically flat, single terminated $LaAlO_3$ (001) substrate surfaces. Ion scattering spectroscopy proves the predominant AlO_x-termination of the atomically flat $LaAlO_3$ (001) surfaces.

[1] A. Biswas, et al., Prog. Surf. Sci. 92, 117 (2017).
[2] H. Y. Hwang, et al., Nat. Mater. 11, 103 (2012).
[3] A. J. H. van der Torren, et al., Phys. Rev. B 91, 245426 (2015).

Effect of Ti stoichiometry on crystal and electronic structure of single crystalline epitaxial $Ba_{0.5}Sr_{0.5}Ti_{1+y}O_3$

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The tunable dielectric material $Ba_xSr_{1-x}TiO_3$ is commonly used as a functional material for construction of tunable capacitors (varactors) which are key building blocks for various microwave devices such as phase shifters and agile antennas. The functional properties of $Ba_xSr_{1-x}TiO_3$ such as dielectric permittivity, electric tunability, and dielectric losses depend sensitively on its (off-)stoichiometry. In particular, the site occupation at the B-site of the ABO_3 $Ba_xSr_{1-x}TiO_3$ perovskite crystal structure has a critical impact on dielectric losses, i.e. leakage current and Q-factor of the varactors.

The possibility to grow fully epitaxial and single crystalline $Ba_xSr_{1-x}TiO_3$ functional layers on an isostructural electrode material allows to study the effect of Ti off-stoichiometry without the interference of grain boundary effects. Furthermore, in single crystalline matter the intrinsic Ti content can be measured precisely by using techniques like in situ X-ray photoelectron spectroscopy (XPS).

Here we present the results of a study of $Au/Pt/Ba_{0.5}Sr_{0.5}Ti_{1+y}O_3/SrMoO_3$ varactors, in which the $Ba_{0.5}Sr_{0.5}Ti_{1+y}O_3$ films have been grown onto highly conducting oxide $SrMoO_3$ bottom electrodes with a room-temperature resistivity below 30 $\mu\Omega$cm [1,2]. The study allows a thorough correlation of thin film synthesis parameters, crystal and electronic structure, and functional device properties

[1] A. Radetinac *et al.*, *Highly conducting $SrMoO_3$ thin films for microwave applications*, Appl. Phys. Lett. **105**, 114108 (2014).

[2] A. Radetinac *et al.*, *Growth and interface engineering in thin-film $Ba_{0.6}Sr_{0.4}TiO_3/SrMoO_3$ heterostructures*, J. Cryst. Growth **463**, 134 (2017).

Understanding the semimetallic state of $SrIrO_3$ thin films: from epitaxial growth to thermal and magneto-transport studies

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As opposed to their $3d$ counterpart, $5d$ transition metal oxides are generally characterized by stronger spin-orbit coupling and weaker correlation effects, resulting in a delicate balance of competing effects having similar energy scales. The interplay between these electronic properties and lattice distortions has recently drawn attention and $SrIrO_3$ was proposed as a candidate topological (semi)metal [1]. Due to its chemical instability in single crystal form, the synthesis of high-quality thin films is essential to advance the exploration of the intriguing physical properties of $SrIrO_3$.

We discuss key issues related to the growth and stability of $SrIrO_3$ thin films on $SrIrO_3$ substrates, paying particular attention to the prevention of degradation of the transport properties in ambient conditions. Our optimization of the lithographic processing allowed the successful fabrication of devices such as Hall bars, suitable to perform quantitative transport characterization in $SrIrO_3$ thin films[2]. We investigated the multi-band nature of this correlated semi-metal by combining magneto-transport, thermoelectric and field-effect measurements, which enabled us to determine the transport coefficients of both holes and electrons[3]. We further elucidate the role of dimensionality in the ultra-thin limit, observing the onset of a metal-insulator transition below a critical thickness of 4 unit cells. Below this thickness, we find the opening of a gap in the density of states, and the on-set of magnetic fluctuations observed in magneto-transport[4].

[1] J.-M. Carter, V. V. Shankar, M. A. Zeb, and H.-Y. Kee, Phys. Rev. B 85, 115105 (2012)
[2] D. J. Groenendijk, N. Manca, G. Mattoni, L. Kootstra, S. Gariglio, Y. Huang, E. van Heumen, and A. D. Caviglia, Appl. Phys. Lett. 109, 041906 (2016)
[3] N. Manca, D. J. Groenendijk, I. Pallecchi, C. Autieri, L. M. K. Tang, F. Telesio, G. Mattoni, A. McCollam, S. Picozzi, and A. D. Caviglia, Phys. Rev. B 97, 081105 (2018)
[4] D. J. Groenendijk, C. Autieri, J. Girovsky, M. C. Martinez-Velarte, N. Manca, G. Mattoni, A. M. R. V. L. Monteiro, N. Gauquelin, J. Verbeeck, A. F. Otte, M. Gabay, S. Picozzi, and A. D. Caviglia, Phys. Rev. Lett. 119, 256403 (2017)

Tailoring Vanadium Dioxide Thin Film Orientation by $Ti_{0.87}O_2$ and $NbWO_6$ Nanosheets

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Vanadium dioxide (VO_2) has been drawing attention since its metal-insulator transition (MIT) with several orders of magnitude resistivity change at 341 K was discovered.[1] The MIT is accompanied with the abrupt first order structural phase transformation from a metallic tetragonal rutile (R) phase (P42/mnm), to an insulating monoclinic (M1) phase (P21/C). Up to now, most studies on epitaxial VO_2 thin films used Al_2O_3 and TiO_2 single crystal substrates to control film orientation. However, VO_2-based devices are restricted to low cost and size-limited single crystal substrates, as well as on the integration compatibility with the current Si-based technology. Direct deposition of VO_2 on glass or Si substrates with a native amorphous silicon dioxide layer leads to a polycrystalline film with predominant $(011)_{M1}$ orientation,[2] whereas VO_2 is favorably grown $(010)_{M1}$-oriented on a buffer layer of Pt(111) on Si substrate.[3] It is worth noting that epitaxial yttria-stabilized zirconia, YSZ(001), on Si(001) can be used to epitaxially grow VO_2 with $(010)_{M1}$ orientation,[4] which enables its integration with Si-based technology.

However, the orientation of VO_2 is limited by the preferential natural growth on amorphous silicon dioxide and limited buffer layers on Si substrates. The challenge is how to direct VO_2 film orientation on Si or even arbitrary substrates at will. Oriented growth is not only of interest for the fundamental study of the MIT mechanisms,[5] but also for potential applications for next-generation transistors,[6] and memory metamaterials.[7] Recently, metal oxide films were grown by epitaxy on oxide nanosheets on Si substrates.[8] Oxide nanosheets are essentially two dimensional (2D) single crystals with a thickness of a few nanometers and a lateral size in the range of micrometers. They span a wide range of crystal lattices and 2D symmetric structures, allowing for new possibilities to tailor the important structural parameters and properties of thin films. Therefore, the choice of substrate becomes a tool of engineering and application.

Tailoring the VO_2 film orientation by nanosheets will be presented.[9] $Ti_{0.87}O_2$ (TO) and $NbWO_6$ (NWO) nanosheets were identified to direct the orientation of VO_2 thin films. Monolayers of nanosheets were deposited on Si substrates by the Langmuir-Blodgett method. Utilizing pulsed laser deposition, single phase VO_2 thin films were grown epitaxially on TO and NWO nanosheets with $(011)_{M1}$ and $(-402)_{M1}$ orientation of the low temperature monoclinic M1 phase, corresponding with $(110)_R$ and $(002)_R$ of the high temperature rutile phase, respectively. Across the MIT, structural changes in VO_2 films were confirmed by X-ray diffraction and the film resistance was measured as a function of temperature. To emphasize the high degree of control over crystallographic VO_2 film orientation, two different orientations were arranged into an alternating line pattern by employing both TO and NWO nanosheets on a single substrate using lithography tools. Interestingly, the different orientations also lead to a difference in the MIT temperature, allowing the on-chip tunability of electronic properties of VO_2.

[1] J. B. Goodenough, J. Solid State Chem. 1971, 3, 490.
[2] J. Jian et al., J. Appl. Phys. 2013, 114, 244301.
[3] J. Sakai et al., J. Appl. Phys. 2013, 113, 123503.
[4] A. Gupta et al., Appl. Phys. Lett. 2009, 95, 111915.
[5] V. R. Morrison et al., Science 2014, 346, 445.
[6] M. Nakano et al., Nature 2012, 487, 459.
[7] T. Driscoll et al., Science 2009, 325, 1518.
[8] M. Nijland et al., Adv. Funct. Mater. 2015, 25, 5140.
[9] T.P.P. Le et al., in preparation.

Thickness dependence of electronic properties in $SrIrO_3$ thin films grown by sputtering

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Strontium Iridates Ruddlesden-Popper (RP) series ($Sr_{n+1}Ir_nO_{3n+1}$) have recently been studied as a playground for studying spin-orbit physics due to the heavy 5d Ir-element. Electronic properties are controlled by a subtle balance between charge, spin and correlation leading to exotic physical properties as the formation of novel Jeff=1/2 and Jeff=3/2 states. Among the different compounds of the RP family, epitaxial stabilized perovskite-like $SrIrO_3$ (n=infinite) raised interest as a narrow-band semimetal close to a Mott insulating transition (MIT). Furthermore, MIT may be triggered by tuning the film thickness of the strain state (compressive). Although growth of thin films of the RP series have been achieved by different techniques as Pulsed Laser Deposition or Molecular Beam Epitaxy, their preparation by sputtering has been challenging and only the n=inf phase has been reported [1].
In this work we present a study on the growth of $SrIrO_3$ thin films by reactive rf sputtering on top of (001)-oriented $SrTiO_3$ and $NdGaO_3$ substrates. We have explored the thermodynamic phase diagram (T-PO_2) to understand the growth and stability of the $Sr_{n+1}Ir_nO_{3n+1}$ phases. Compositional analysis in combination with transmission electron microscopy (TEM) images gave us insights into the nucleation processes during sputtering. Optimal conditions to growth high quality $SrIrO_3$ thin films were thus achieved. Magnetotransport properties (magnetoconductivity and Hall effect) were studied as a function of film thickness and strain. The results will be discussed in terms of dimensionally enhanced Mott insulator transition.

[1] L. Fruchter, O. Schneegans and Z.Z. Li, Journal of Applied Physics 120, 075307 (2016)

Multi Process Thin Film Deposition and complex Sample Preparation Cycle under protected Atmosphere

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New materials or advanced functional films are always dedicated for specific aplications. Very often either the substrate material or the film material are strongly sensitive against normal environmetal conditions. Even if the components of such deposition are not sensitiv against such attac, the interfacing between substrate and film is effected from such influence. The solution in material research for such problems is an isolation of such substrate under strongly controlled atmosphere, which can be achieved with the use of glove boxes with integrated gas cleaning systems. The user interacts via isolation gloves to handle sensitive materials in the glove box wich are introduced to it via integrated load lock ports. The combination of such controlled work bench to any kind of deposition system is a problem, because normally no easy way exist to transfer such materials from a glove box into separate deposition systems. Only a fully protected connection from such glove box to the deposition system allows an undisturbed transfer. But standard deposition systems are not prepared for such transfer. SURFACE offers now fully integrated process systems which have a complete glovebox built in. In addition the complete design of such system recognizes the reduction of handling performance of the user caused by the thick gloves and its limited taktile sensitivities. Any services on such deposition system is generated from the atmosphere side, without disturbing the conditions of the contolled atmoshere in the glove box. The fully integrated style of the glove box reduces also the necessary floor space of such comlete set-up in the lab. As an excample : the total foot print of a complet PLD Glove Box system including big Excimer laser, its gas cabinet, the process automation system with user interface, the vacuum chamber, cooling chiller and the gas control cabinet fits to a floor space of 2,5 m x 0,8 m and includes already the glove box workstation with a working width of 1 to 1,5 m. Examples for such integrated systems are presented.

Realization of freestanding transition metal oxide 2D crystals of sub-nanometer thickness

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The rich fundamental science and emergent applications discovered in conventional 2D systems have inspired the search of their strongly correlated analog in transition metal oxides for years but hindered by the extremely difficult sample preparation. Recent breakthrough in synthesizing freestanding oxide films of high crystalline quality using water soluble $Sr_3Al_2O_6$as the sacrificial buffer layer[1] sheds light on the artificial design of 2D crystals out of vast amount of complex oxides, even including those of three dimension in nature in their bulk form. However, Seung et al. recently demonstrated that $SrTiO_3$membrane lattice collapses below a critical thickness of 5 unit cell (u.c.) and proposed an inherent thickness limit of oxide crystals based on the continuum elastic theory and Berezinskii-Kosterlitz-Thouless (BKT) model[2]. For films thicker than this BKT limit, the electronic structure is 3D like, which impedes the realization of truly 2D correlated electrons in transition metal oxides. Here, we report the overcoming of the BKT limit and the realization of high-crystalline-quality 2D transition metal oxide crystals of sub-nanometer thickness. In the 2D limit, the prominent asymmetry between the in-plane and out-of-plane bonding conditions results in an abnormally large c/a ratio and giant polarization in the case of $BiFeO_3$. In addition to providing a fertile field of 2D correlated phases, the capability of integrating high-crystalline-quality ultrathin oxide 2D crystals on any substrates enables the direct incorporation of superior strongly correlated properties in conventional semiconductors, paving the way for a new generation of multifunctional electronic devices.

[1] Lu, D. et al., Nature materials 15, 1255 (2016)
[2] Hong, S. S. et al., Science advances 3, eaao5173 (2017)

Large area PLD of ferroelectric oxides on silicon for neuromorphic applications

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Inspired by the biological architecture of the brain and with the goal to mimic the processes underlying learning and memorization, we are developing memristive ferroelectric tunnel junctions (FTJs) for applications in neuromorphic computing, which allows for highly energy efficient and massively parallel data processing and storage.

FTJs are non-volatile memory devices with non-destructive readout whose resistance can be tuned by polarization reversal of a nanometer-thick ferroelectric layer sandwiched by two dissimilar metallic electrodes. Recently, several groups demonstrated the possibility to continuously tune the resistance of FTJs between the ON and OFF state [1,2]. Such memristive behavior is the key to mimic synaptic behavior in artificial neural networks and is realized through partial polarization switching of nanodomains within a single FTJ device [3].

For actual applications of complex oxides and industrial feasibility it is important to upscale sample fabrication processes from the millimeter to the wafer scale. To this end, a custom-made large area pulsed laser deposition (PLD) system is used to grow layers with atomically well-defined, sharp interfaces, which is a prerequisite for FTJs.

PLD parameters are optimized to grow ultrathin lead-free ferroelectric oxides, $BiFeO_3$ and $BaTiO_3$, and conducting $LaNiO_3$ bottom electrode layers on 2 inch $SrTiO_3$ buffered Si wafers [4]. AFM, XRR, and XRD are used to confirm the required flatness of less than 1 nm peak-to-peak roughness and epitaxy, respectively. Co/Au contact pads defined by conventional UV lithography,sputtering, and lift-off techniques are used as top electrodes for mesoscale electrical measurements and compared with nanoscopic PFM data to prove ferroelectricity in the ultrathin limit.

Future work includes the fabrication of crossbar arrays and their integration with CMOS, eventually demonstrating machine learning capabilities such as pattern recognition in hardware and interfacing the system with complex signals such as the output of an event-based camera [5].

[1] Chanthbouala, A. et al. A ferroelectric memristor. Nat Mater 11, 860-864 (2012)

[2] Kim, D. J. et al. Ferroelectric tunnel memristor. Nano Lett. 12, 5697-5702 (2012)

[3] Boyn, S. et al. Learning through ferroelectric domain dynamics in solid-state synapses. Nat. Commun. 8, 14736 (2017)

[4] Norga, G.J. et al. Phase of reflection high-energy electron diffraction oscillations during (Ba,Sr)O epitaxy on Si(100): A marker of Sr barrier integrity. Appl. Phys. Lett. 87, 262905 (2005)

[5] http://www.ulpecproject.eu

Magnetic anisotropy and spin dynamics in chemically deposited $La_{0.92}MnO_3$ thin films

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The electronic and magnetic properties of perovskite oxides are known to be extremely dependent on small compositional deviations that change the nature and valence states of B-site ions. This is particularly important in the case of $LaMnO_3$ (LMO), the parent compound of the colossal magnetoresistance manganite family. In its bulk stoichiometric state, LMO is an insulating antiferromagnetic material due to the strong cooperative Jahn-Teller effect. Nevertheless, the presence of cationic vacancies gives rise to a mixed-valence Mn leading to a conducting ferromagnetic behavior typical of double-exchange mechanism. This behavior converts La-deficient LMO in a potential candidate for spin current generation. In spite of this interest, there is scarcy literature on this compound, as the controlled preparation of cationic deficient LMO thin film is a challenging task because the transfer of target stoichiometry into the film is strongly dependent on growth conditions [1]. This issue is solved by chemical deposition methods where stoichiometry is easily controlled by the right ratio of precursor solutions.

In this work, we present a study of the magnetic properties of La-deficient $LaMnO_3$ thin films grown by polymer assisted deposition (PAD) method. The metal nitrate precursors were dissolved in an aqueous solution of Polyethylenimine and Ethylenediaminetetraacetate and then spin coated on (001)-oriented $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) substrates. Thermal treatments were optimized to obtain thin films with a high quality terraced surface morphology suitable to study interfacial effects.

Temperature dependent magnetic properties were measured by using broadband microstrip ferromagnetic resonance (FMR). Angular measurements showed the presence of an important in-plane magnetic anisotropy with [110] as the easy-axis. We have also studied the influence of strain in the spin dynamics. Magnetic Gilbert damping was determined from the frequency dependence of the FMR linewidth. We will show that different damping parameters are obtained for films grown on top of LAO and STO substrates. Our results show that La-deficient LMO thin films grown by chemical methods are potential candidates for spin pumping devices.

[1] I Marozau et al., Physical Review B 89, 174422 (2014)

Giant Electrostatic Modification of Magnetism via Electrolyte-Gate-Induced Cluster Percolation in Epitaxial $La_{1-x}Sr_xCoO_3$

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Recently, electrolyte gating techniques using ionic liquids have proven highly effective in tuning large carrier densities at material surfaces. These electrolytes enable electric double layer transistor operation, the large capacitances (10's of $\mu F/cm^2$) generating electron/hole densities up to 10^{14} - 10^{15} cm^{-2}, i.e., significant fractions of an electron/hole per unit cell in most materials. Uncertainties remain, however, including the true doping mechanism (i.e., electrostatic vs. electrochemical), the challenge of in operando characterization, and the need to understand the full potential and universality. In our work we have focused on the use of ionic gels, in all-solid-state devices, enabling gate-control of ferromagnetism. Employing epitaxial $La_{1-x}Sr_xCoO_3$ as a model system, our findings first clarified charge carrier vs. oxygen defect creation. Dramatic asymmetry with respect to bias polarity was observed in both transport [1] and in operando synchrotron X-ray diffraction and polarized neutron reflectometry (PNR) [2]. In essence, we find oxygen vacancy formation at positive bias, but electrostatic hole accumulation at negative bias, which can be interpreted in a simple picture where electrostatic vs. electrochemical response is dictated by enthalpy of formation and diffusivity of oxygen vacancies, and bias polarity [1,2]. Control of ferromagnetism is then possible in both electrochemical [2] and electrostatic [1] modes. In this talk we focus in particular on purely electrostatic operation, at negative bias. Guided by recent theory [3] we demonstrate large enhancement of electrostatic changes in ferromagnetic order by thickness tuning to the brink of a percolation transition [4]. Application of only -3 V then drives a transition from a short-range-ordered insulator to a long-range ferromagnetic metal, thus realizing giant electrostatic Curie temperature modulation over a 150 K window [4]. This is the largest unambiguous electrostatic TC shift yet obtained in any electrolyte-gated system or in any complex oxide, by any means. In operando PNR confirms gate-controlled ferromagnetism, additionally demonstrating anomalously deep penetration of induced magnetization, well beyond the Thomas-Fermi screening length [4]. This latter result will be discussed in terms of recently-developed theory [3].

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[1] Walter et al., ACS Nano 10, 7799 (2016).
[2] Walter et al., Phys. Rev. Mater. 1, 071403(R) (2017).
[3] Orth et al., Phys. Rev. Lett. 118, 106801 (2017).
[4] Walter et al., submitted, (2018).

Resonant control of magnetism via selective excitation of the lattice vibration in magnetic oxide $DyFeO_3$

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The exploitation of ultrashort (<100 fs) pulses of light to control electronic and magnetic properties of solids is an emerging area with potential to impact information processing technology. Recent advances in laser sciences enable the generation of broadly tunable ultrashort mid-infrared light pulses with peak fields reaching values of 10 MeV/cm. These pulses selectively tuned in resonance with specific phonon modes of a crystal can stimulate coherent perturbation of the lattice and were shown to drive metal-insulator transitions, perform coherent control of magnetism, or even enhance the superconductivity on the ultrafast timescale.

Here we explore how resonant pumping of the Fe-O stretching mode influences the magnetic state of the antiferromagnetic insulator $DyFeO_3$. We perform a time-resolved all-optical pump probe experiment and demonstrate that the excitation establishes transiently a new orientation of the spins and launches high-amplitude spin precession around the new equilibrium. Considering the substantial shift (∼20 %) of the resonance frequency it altogether evidences a strong modification of the magnetic potential caused by the lattice perturbation. We attribute these results to the lattice-driven modulation of the anisotropic exchange interaction between Dy and Fe ions effectively seen as changes in the magnetic anisotropy. Establishing a direct link between the lattice excitation and the modification of the anisotropic exchange is the key point of the present work.

Non-local Detection of Spin diffusion in $LaAlO_3/SrTiO_3$ Heterostructures

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A plethora of exciting properties have been observed at the oxide heterointerface between $LaAlO_3$ and $SrTiO_3$. Most prominently it has been demonstrated that the confined electron gas formed at the interface features e.g. gate-tunable superconductivity, ferromagnetism and a sizeable Rashba spin-orbit coupling. This Rashba spin-orbit coupling allows a considerable charge/spin interconversion to take place at this particular interface as previously demonstrated by spin pumping ferromagnetic resonance experiments from a NiFe contact [1]. Moreover, the efficiency of this charge-to-spin conversion was amazingly even demonstrated to be gatable. Transport experiments of patterned $LaAlO_3/SrTiO_3$ devices have also allowed detection and quantification of this charge-to-spin conversion through non-local resistance measurements [2]. Here, we perform such Hanle measurements of the non-local resistance in patterned amorphous-$LaAlO_3/SrTiO_3$ devices. Specifically, we investigate the temperature dependence of the non-local resistance as well as its dependence with magnetic field direction. From these measurements, we extract the spin Hall angle and characteristic spin diffusion length at 2 K to be 0.17 and 750 nm, respectively.

[1] E. Lesne et al. Highly efficient and tunable spin-to-charge conversion through Rash-ba coupling at oxide interfaces. Nature Materials 15, pages 1261-1266 (2016).
[2] M.-J. Jin et al. Nonlocal Spin Diffusion Driven by Giant Spin Hall Effect at Oxide Heterointerfaces. Nano Letters 17, 36 (2016).

Reversible magnetoelectric switching by electrochemical lithium intercalation

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We are working on a method to observe the relation between charge ordering and magnetism in manganites ($A^{3+}_{1-x}B^{2+}_{x}MnO_3$). These have complex phase diagrams as a function of composition x and temperature T with a variety of magnetic and electronic phases. $La_{1-x}Sr_xMnO_3$ (LSMO) shows transitions between ferromagnetism (FM) and paramagnetism at room temperature and between antiferromagnetism (AFM) and FM at lower T for x = 0.5. It is believed that the driving force is the ordering of Mn^{3+} and Mn^{4+}, which sets in at x = 0.5. [1] Our approach is to reversibly[2] change the Mn^{3+} / Mn^{4+} ratio by de-/lithiating the material electrochemically, using a Li-ion battery-like half-cell and to monitor the process in-situ. In addition to LSMO we use the already lithiated material $La_xSr_yLi_zMnO_3$ (LSLMO) starting on the FM-side of the phase boundary. Polarized Neutron Reflectometry (PNR) gives insight to the lithium distribution and the magnetic induction profile within the manganite layers. The reversibility[2] of the process allows us to investigate the same sample in various states around the phase transitions and thus will help to resolve the contributions to the phase formation and to quantify their mutual connection.

Samples of various compositions were grown by Pulsed Laser Deposition and characterized structurally and electrochemically. To determine the magnetic states of the samples, PNR measurements were carried out at room T as well as down to 100 K on Amor. For the in-situ PNR measurements an electrochemical cell was designed and built. The first measurements qualitatively showed that magnetic switching is possible for LSLMO and gave hints that also LSMO undergoes the phase transition.

[1] E. Dagotto et al., Physics Reports 344, 1 (2001)
[2] S. Dasgupta et al., Advanced Materials 26, 4639 (2014)

Axial spin-momentum locking and valley degree of freedom in antiperovskite Dirac materials

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In 3D Dirac/Weyl semimetals, chirality (pseudospin) is known to govern their exotic physics. However, in general, real spin could also contribute to physical phenomena due tosizable spin-orbit coupling in these materials. We aimed at disentangling the role of pseudospin and spin in a Dirac material Sr3SnO, by analyzing the valley degree of freedom in quantum interferencepart of magnetotransport.Our results point to a dominant role of real spin, which we attribute to a spin-quantization axis locking found in eachDirac pocket. We discuss how this could lead to a rapid spin rotation when E_F is close tothe Dirac point. In the presentation, I will also describe some details on the molecular beam epitaxy (MBE) growth of antiperovskites which we have developed recently [1].

[1] D. Samal, H. Nakamura, and H. Takagi., APL Mater. 4, 076101 (2016)

Analysis of magnetic anisotropy on in artificially multiferroic $BaTiO_3/La_{2/3}Sr_{1/3}MnO_3$ heterostructures

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In multiferroic heterostructures magnetoelectric coupling between a ferroelectric and a ferromagnetic material has been extensively studied as promising routes towards electric field controlled magnetism. In this work, we report the magnetic anisotropy in strain-coupled systems. In strain-coupled systems, direct correlations between the polarization direction within ferroelectric domains and the locally-induced magnetic anisotropy have been demonstrated [1-2]. We have deposited bilayers of the FM $La_{2/3}Sr_{1/3}MnO_3$ and FE $BaTiO_3$ as a possible route to design systems with artificial magnetoelectric coupling on BTO/LSMO on STO substrate. We maintain a fixed ferroelectric layer thickness (t_{BTO}= 140 nm) and ferromagnetic layer (t_{LSMO} = 25 nm). We analyze the substrate direction influence on electrical and magnetic properties of manganite. From XRD we found that the BTO layer for STO(001) growth textured with almost two different distribution of domains (c domains in plane and out-plane) with c_{BTO}=4.108 Å and LSMO layer growth textured with c_{LSMO}=3.855 Å. Interestingly, for STO(110) and STO(111) the BTO layer and LSMO layer the growth is textured (only c domains out plane) with c_{BTO}=4.037 Å and c_{BTO}=4.018 Å while LSMO growth is also textured with c_{LSMO}=3.867 Å and c_{LSMO}=3.858 Å, respectively. Magnetization with temperature curves shows a ferromagnetic transition for all bilayers at room temperature with a magnetization between 280-320 emu/cm^3. Measures of anisotropy of Isothermal hysteresis loops at 300 K show a change in magnetic anisotropy for bilayer growth on STO(001) from biaxial magnetic ordering (LSMO/STO(001)) to uniaxial magnetic ordering (bilayer), probably due to BTO layer influence on magnetic properties on LSMO layer. However, for other substrates direction this behavior is not observed, indicating the possible influence of c domains in plane in this change on magnetic anisotropy. This effect has not been observed in the bilayers grown on LSAT and LAO substrates. This result revealed that the superficial strain effect only induced a uniaxial anisotropy when the LSMO film was grown with a tensile strain. Ferroelectric properties on BTO at room temperature, shows a polarization saturation between 20-40 μC/cm^2. This work has been supported by Instituto de Nanociencias de Aragón, Zaragoza, Spain, where the films were grown and partially characterized and Center of Excellence on Nobel Materials-CENM, research projects: CI7917-CC 10510 COLCIENCIAS and CI 7978 UNIVALLE.

[1] Y.-H. Chu et al., Nature Materials, 7, 478 (2008).

[2] R. Streube et al., Phys. Rev. B 87, 054410 (2013).

Paramagnetic to antiferromagnetic quantum critical phase transition induced by bandwidth reduction

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Four paramagnetic non-Fermi liquid (NFL) perovskite oxides with varying B-site cations across the d-block of periodic table, namely: $LaNiO_3$, $CaRuO_3$, $CaIrO_3$ and $SrIrO_3$, are found to show consistent evidence of paramagnetic to antiferromagnetic phase transition, as their localization regime was reached. In the bulk, these materials are classified as the "resilient quasiparticle (RQP) phase" above the Quantum Critical Point (QCP) in a universal phase diagram of temperature versus correlation factor (U/t). They also in the magnetic fluctuation state due to small Hund's coupling and large bandwidth. Here we present two ways to force a paramagnetic (PM) to antiferromagnetic (AF) transition among the mentioned materials: (1) by thinning down the materials to their carrier localization regime, and (2) by growing them into a superlattice separated by STO spacers: $[\text{PM (1uc)} + \text{STO (1uc)}]_{x20}$. These samples showed consistent behaviours of fourfold symmetric oscillation in in-plane anisotropic magnetoresistance (IP-AMR) reflecting a cubic biaxial magnetocrystalline anisotropy; as well as clear Neel temperatures (T_N) at large field in magnetometry due to AF spin-flop. This work thus presents a convincing experimental depiction of the quantum critical phase transition.

[1] D. Yi et al., Proceedings of the National Academy of Sciences (Supplementary Information) 113, 6397 (2016)
[2] J. Matsuno, K. Ihara, S. Yamamura, H. Wadati, K. Ishii, V. V. Shankar, H.-Y. Kee, and H. Takagi, Phys. Rev. Lett. 114, 247209 (2015)
[3] S. Tripathi, R. Rana, S. Kumar, P. Pandey, R. S. Singh, and D. S. Rana, Sci. Rep. 4, 3877 (2014)
[4] R. Scherwitzl, S. Gariglio, M. Gabay, P. Zubko, M. Gibert, and J. M. Triscone, Phys. Rev. Lett. 106, 246403 (2011)

Double-perovskite La_2NiMnO_6: a thin film and a superlattice approach

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Epitaxial heterostructures offer multiple approaches to manipulate the interplay between the different degrees of freedom in transition metal oxides. Strain and reduced dimensionalities are examples of successful strategies typically used to tune the functionalities of these materials and even allow access to novel electronic phases.
The double-perovskite La_2NiMnO_6 is well studied in bulk due to its near room temperature ferromagnetic transition (T_c 280K), accompanied by magnetoresistance and magnetoelectric effects [1]. Here, we tackle two different heterostructure strategies to investigate such double-perovskite. First, we investigate the electronic properties of La_2NiMnO_6 when grown as thin film, focusing on the thickness- and strain-dependence of the ferromagnetic behaviour. Second, we look at $(111)_{pc}$-oriented $LaNiO_3/LaMnO_3$ superlattices, since they allow to reproduce the double-perovskite structure when periodicities of 1u.c./1u.c. are chosen. In this case, the electronic properties of the system are investigated as function of the superlattice periodicity. For 7-monolayer-thick-$LaNiO_3$, low-temperature exchange bias phenomena followed by interlayer antiferromagnetic coupling between $LaMnO_3$ layers is observed as function of temperature [2,3].

[1] N. S. Rogado et al., Adv. Mater. 17, 2225 (2005).
[2] M. Gibert, et al., Nat. Mater. 11, 195 (2012).
[3] M. Gibert et al., Nat. Commun. 7, 11227 (2016).

Structural and electronic properties of rare-earth vanadate heterostructures

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Rare earth vanadates (RVO3) have a rich phase diagram with two different spin and orbital orders depending upon the size of the lanthanide rare-earth cation (i.e. R) [1]. Of these, yttrium vanadate is particularly interesting, exhibiting two different kinds of spin and orbital orders and phenomena such as temperature induced magnetization reversal [2]. Heterostructuring these materials alters their structure through epitaxial strain and could further introduce spatial confinement and interface effects [3]. The consequential changes in their electronic properties is of interest here.
Films and multilayers of yttrium vanadate (YVO3) with LaAlO3 were grown using ultra-high vacuum pulsed laser deposition (UHV-PLD) on NdGaO3 substrate.X-ray diffraction (XRD) and scanning transmission electron microscopy (STEM) were used for structural characterization of the samples. In particular, the determination of the unit cell orientation with respect to the substrate was done using XRD, which is crucial for polarization dependent x-ray studies.Resonant elastic x-ray scattering (REXS) was used to obtain depth resolved information about the electronic structure of YVO3 in the multilayers [3], which revealed a modulation of scattering factors through the YVO3 layers which may indicate a difference in orbital polarization or the charge on the vanadium ion across the depth.

[1] S. Miyasaka, Y. Okimoto, M. Iwama, and Y. Tokura. Spin-orbital phase diagram of perovskite type RVO3. Phys.Rev.B, 68, 2003.
[2] H.Hwang, et.al. Emergent phenomena at oxide interfaces. Nature Materials, pages 103-113 (2012)
[3] Y. Ren, et.al. Magnetic properties of YVO3 single crystals. Phys. Rev. B, 62, (2000)
[4] E. Benckiser et.al. Orbital reflectometry of oxide heterostructures. Nature Materials, 10, (2011)

Controlling magnetization in $SrTiO_3$ quantum wells embedded within Mott insulating heterostructures

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Engineering thin film interfaces remains one of the strongest strategies to generate functional electronic and magnetic properties in materials. Strongly correlated materials, such as complex transition metal oxides, are particularly well suited to this approach because the tight competition between their various energy scales (e.g. strain, electronic bandwidth, magnetic exchange) often leads to multiple proximate ground states that can be easily tuned. We have studied thin film heterostructures containing quantum wells of the band insulator $SrTiO_3$ embedded within a Mott insulating rare earth titanate $RTiO_3$ (R = Gd, Sm) matrix. At the $RTiO_3/SrTiO_3$ interface, electrostatic doping creates a high-density two-dimensional electron liquid (2DEL) that resides within the $SrTiO_3$ layers near the interface, and hosts a metal-to-insulator transition or quantum criticality depending on the choice of neighboring Mott layer. We used a combination of polarized neutron reflectometry and low-energy muon spin rotation to probe magnetism in the buried layers of these heterostructures. Our results show that there is a critical well thickness of 2 nm, below which the 2DEL electrons within these thin $SrTiO_3$ layers exhibit robust, magnetic correlations. This critical thickness is independent of the neighboring Mott layers' magnetic exchange interaction. However, the magnetic correlations exhibited by the embedded $SrTiO_3$ wells track that of the host matrix. Namely, $SrTiO_3$ within ferrimagnetic $GdTiO_3$ displayed ferromagnetic behavior, while $SrTiO_3$ embedded within antiferromagnetic $SmTiO_3$ showed evidence of antiferromagnetic correlations. Finally, in the case of a $SmTiO_3$ matrix, the onset of antiferromagnetic correlations in the $SrTiO_3$ well coincides with the opening of a pseudogap in the tunneling spectra and results in a quantum critical phase space reminiscent of unconventional superconductors. Together, these studies add to our collective understanding of electron-electron correlations in complex oxides with high-density 2D electron systems.

The role of atomic reconstructions and antiferromagnetic spin structure to establish emerging interface spin textures at the (111)-oriented $La_{0.7}Sr_{0.3}MnO_3/LaFeO_3$interface

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The nearly degenerate ground states of competing order in oxide heterostructures allow for strain engineering to control interface functionality. A central question is which role structural reconstructions and inherent spin structure play to establish new magnetic spin textures. To address this question (111)-oriented epitaxial heterostructures of antiferromagnetic (AF) $LaFeO_3$ (LFO) and ferromagnetic $La_{0.7}Sr_{0.3}MnO_3$(LSMO)are used as model system, and we present data on the interplay between AF spin axis of LFO and the occurrence of magnetic reconstructions at the (111)-oriented LSMO/LFOinterface. To probe the interface spin texture, we rely on a combined soft x-ray spectroscopy, neutron reflectometry, and DFT investigation. By increasing the LFO thickness, a change from out-of-plane to in-plane AF spin axis takes place above 16 d111-layers, below which a magnetic interface reconstruction with a net switchable Fe momentof LFO is observed when deposited of $SrTiO_3$. By using orthorhombic substrates, the anisotropy of the magnetically reconstructed interface can be controlled, from 6-fold when deposited on $SrTiO_3$ to 2-fold. Moreover, by performing hysteresis measurements, the of role exchange coupling between LSMO and LFO is elucidated. The data will be discussed in the context of the interplay between anisotropic strain and a successively decreased out-of-plane canting of the AF spin axis towards the in-plane LSMO magnetization at the interface. Taken together the data point towards the importance of the interplay between local AF order and concurrent structural reconstructions to establish a magnetically reconstructed interface, opening for tuning the AF-spin texture by interface engineering.

Origin of Emergent Ferromagnetism in Otherwise Antiferromagnetic $LaMnO_3$ Thin Films

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Atomically engineered oxide heterostructures provide a fertile ground for creating novel states.[1] For example, a two-dimensional electron gas at the interface between two oxide insulators, giant thermoelectric Seebeck coefficient, emergent ferromagnetism from otherwise nonmagnetic components, and colossal ionic conductivity. Extensive research efforts reveal that oxygen deficiency or lattice strain play an important role in determining these unexpected properties.[2,3] Herein, by studying the abrupt presence of robust ferromagnetism (up to 1.5 μ_B/Mn) in $LaMnO_3$-based heterostructures, we find the multivalence states of Mn that play a decisive role in the emergence of ferromagnetism in the otherwise antiferromagnetic $LaMnO_3$ thin films. Combining spatially resolved electron energy-loss spectroscopy, X-ray absorption spectroscopy and X-ray magnetic circular dichroism techniques, we determine unambiguously that the ferromagnetism results from a conventional Mn^{3+}-O-Mn^{4+} double-exchange mechanism rather than an interfacial effect. In contrast, the magnetic dead layer of 5 unit cell in proximity to the interface is found to be accompanied with the accumulation of Mn^{2+} induced by electronic reconstruction.[4] These findings provide a hitherto-unexplored multivalence state of Mn on the emergent magnetism in undoped manganite epitaxial thin films, such as $LaMnO_3$ and $BiMnO_3$, and shed new light on all-oxide spintronic devices.

[1] H. Y. Hwang, Y. Iwasa, M. Kawasaki, B. Keimer, N. Nagaosa, Y. Tokura, Nat. Mater. 2012, 11, 103.
[2] J. A. Kilner, Nat. Mater. 2008, 7, 838.
[3] J. N. Eckstein, Nat. Mater. 2007, 6, 473.
[4] W. Niu, W. Liu, M. Gu, Y. Chen, X. Zhang, M. Zhang, Y. Chen, J. Wang, J. Du, F. Song, X. Pan, N. Pryds, X. Wang, P. Wang, Y. Xu, Y. Chen, R. Zhang, Adv. Electron. Mater. 2018, 4, 1800055.

Controllable Spin Injection across a Crystalline $BaTiO_3$-Germanium Interface

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The epitaxial integration of functional oxides on conventional semiconductors opens new opportunities for coupling their unique properties with semiconductors for post-CMOS technologies. Here we demonstrate an electrically controllable spin-injection device based on epitaxial $BaTiO_3$ on Ge (001) heterostructures. Guided by a numerical analysis of the charge transport, we first show spin accumulation in the p-type Ge with a spin lifetime τ_{sf} 10^2 ps, longer by two orders of magnitude than previous results. We find via analytical calculations that this long τ_{sf} is enabled by Fowler-Nordheim (F-N) tunneling of spin-polarized minority carriers into the Ge conduction band and is limited by short-range core-potential-mediated electron-ionized impurity scattering for 150 K $<$ T $\leq$ 250 K. The spin resistance-area product, which is a measure of spin injection, agrees quantitatively with estimated spin accumulation in the Ge for the highest measured injection currents. We also demonstrate control of the spin signal by manipulating the band profile across the heterojunction, which modulates the charge transport between impurity-assisted conduction and F-N tunneling, effectively acting as a "switch" for spin injection. This approach points to a new paradigm of spin-dependent phenomena in semiconductor-based tunnel devices via band profile tuning.

Intrinsic magnetism of Aurivillius-type multiferroic thin films probed by resonant inelastic X-ray scattering and polarized neutron reflectivity

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Unambiguous magnetic characterization of room-temperature multiferroic materials remains challenging due in part to the difficulty of distinguishing their very weak ferromagnetism from magnetic impurity phases and other contaminants. In this study, the $Bi_6Fe_2Ti_3O_{18}$, $Bi_6FeCoTi_3O_{18}$, and $LaBi_5FeCoTi_3O_{18}$ Aurivillius-type multiferroic epitaxial thin films were prepared. We used resonant inelastic X-ray scattering and polarized neutron reflectivity to probe the electronic structures and magnetizations of the films. The resonant inelastic X-ray scattering measurement reveals the modified crystal-field parameters of FeO_6 and CoO_6 octahedra induced by the doping of Co and La. The polarized-neutron-reflectivity study demonstrates the weak magnetism of the doped Aurivillius oxides and helps to clarify the true mechanism behind the room-temperature magnetic performance.

[1] Z. Cui, X. Zhai, Y.-D. Chuang, H. Xu, H. Huang, J. Wang, Z. Fu, R. Peng, J. Guo, and Y. Lu, Phys. Rev. B 95, 205102 (2017).
[2] X. Zhai, A. J. Grutter, Y. Yun, Z. Cui, and Y. Lu, Phys. Rev. Mater. 2 (2018).
[3] Z. Cui, H. Xu, Y. Yun, J. Guo, Y.-D. Chuang, H. Huang, D. Meng, J. Wang, Z. Fu, R. Peng, R. J. Knize, G. J. Brown, X. Zhai, and Y. Lu, J. Appl. Phys. 120, 084101 (2016).

Electrical properties of $(111)_{pc}$ $SmNiO_3/NdNiO_3$ superlattices

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Rare earth nickelates ($RNiO_3$ (RNO), R = rare earth) stand out for their unique metal to insulator transition (MIT) happening at T_{MI}, accompanied by an unusual antiferromagnetic ordering at $T_{Néel} \leq T_{MI}$ (1-3). In bulk, $NdNiO_3$ (NNO) exhibits $T_{Néel}=T_{MI}$, whereas $SmNiO_3$ (SNO) displays $T_{MI}>T_{Néel}$. It has been shown that the T_{MI} and $T_{Néel}$ of the corresponding films can be tuned over a wide temperature range by means of epitaxial strain (4). Moreover, by selecting orthorhombically-distorted substrates oriented along the (111)pc crystallographic direction, one can induce a splitting of T_{MI} and $T_{Néel}$ of $NdNiO_3$ over a temperature range never achieved for films grown in the (001)pc-orientation (5). Notably, the interfacial matching constraints in the (111)pc direction are much stronger than in the (001)pc direction, therefore the structure of the materials responds differently affecting the electronic properties of the system. Here, we present (001)pc and (111)pc-oriented $(mSmNiO_3/nNdNiO_3)N$ superlattices (SLs). The electronic properties of both heterostructures have been investigated by performing electrical transport measurements and soft x-ray reflectivity measurements.

[1] Catalano et al., Rep. Prog. Phys. 81 046501 (2018)
[2] M. L. Medarde, J. Phys.: Condens. Matter 9, 1679 (1997)
[3] G. Catalan, Phase Transit. 81, (2008)
[4] Catalano et al., APL Materials 2, 116110 (2014)
[5] Catalano et al., APL Materials 3, 062506. (2015)

Laser-ARPES Investigation of the Electronic Structure of $LaNiO_3$ Thin Films

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The ability to grow complex oxide thin films with controlled thicknesses down to a few nanometers offers an opportunity to explore the effect of confinement into strongly correlated electron systems. Here, we present a study of the electronic structure of $LaNiO_3$ thin films by means of angle resolved photoemission spectroscopy (ARPES). We have developed a sputtering apparatus that combines the capabilities of growing high quality oxide heterostructures with the transferring of samples under ultra-high vacuum conditions to a state-of-the-art laser-ARPES setup. Using this combined sputtering-ARPES setup allows us to study the electronic structure of $LaNiO_3$ thin films with unprecedented high resolution. We have measured the Fermi surface and observed electron and hole pocket areas that remain largely unchanged for metallic samples of thickness larger than 15 u.c. consistent with previous findings. As the thickness of the thin films decreases below 15 u.c. we observe a gradual reduction in the electronic mean free path extracted from momentum distribution curve peak widths at the Fermi level. Thin films thinner than 4 u.c. are insulating in transport experiments and present limited spectral weight at the Fermi level at low temperatures.

Ultrahigh-resolution Resonant Inelastic X-ray Scattering from rare-earth nickelates: magnetic and dd-excitations

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Rare-earth nickelates (RNiO$_3$) have been subject to intense investigation, mostly because of the rich phase diagram comprising a sharp temperature-driven metal-to-insulator transition, an unusual antiferromagnetic ground state, and the prospect of mimicking the physics of high-T_c superconducting cuprates in orbitally engineered heterostructures.

We have studied RNiO$_3$ thin-films and superlattices using ultrahigh-resolution resonant inelastic x-ray scattering (RIXS) at the Ni L_3 edge. Below the magnetic ordering temperature, we observe well-defined collective magnon excitations. Our observation provides for the first timean experimental evaluation of the magnetic dynamics in RNiO$_3$ that serves as a solid basis for the theoretical description of their magnetism. In addition to magnetic excitations, we investigated the electronic excitations of RNiO$_3$ as a function of temperature and tolerance factor, *i.e.* rare-earth radius. A sophisticated analysis based on an advanced double-cluster model gives intriguing insight into the microscopic and electronic structure of RNiO$_3$. Our study reveals that RIXS is an excellent technique to simultaniously characterize different ordering phenomena within one material.

[1] Green et al., Phys Rev. B 94, 195127 (2016)

[2] Bisogni et al., Nat. Commun. 7, 13017 (2016)

In Situ TEM of Structural and Resistive Phase Transitions in $La_{2/3}Sr_{1/3}MnO_3$ Driven by Voltage Pulses and Strain

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Oxygen defects can have a profound effect on the physical properties of transition metal oxides. In complex oxides where magnetic, ferroelectric and superconducting phases emerge from strong correlations between localized transition metal valence electrons, oxygen vacancies can radically alter a plurality of intrinsic properties via valance changes and structural phase transitions [1]. The ability to control the concentration and profile of oxygen vacancies in oxide nanostructures would thus open up comprehensive prospects for new functional ionic devices. Advancements in this direction require experimental techniques that allow for simultaneous measurements of oxygen vacancy dynamics, atomic-scale structural effects and macroscopic physical properties.

Here, we use in situ transmission electron microscopy (TEM) to demonstrate reversible switching between uniform structural phases in epitaxial $La_{2/3}Sr_{1/3}MnO_3$ films. In our experiments, we employ a piezo-controlled probing holder to apply short voltage pulses and local strain. Simultaneous high-resolution imaging and resistance probing under zero strain reveals reproducible voltage-induced transformations between a low-resistance perovskite phase, a high-resistance $La_{2/3}Sr_{1/3}MnO_{2.5}$ brownmillerite structure, and an intermediate-resistance perovskite-like phase [2]. Reversible horizontal migration of oxygen vacancies within the manganite film, driven by combined effects of Joule heating and bias voltage, predominantly triggers the structural and resistive phase transitions. Concurrent application of perpendicular strain and voltage pulses produces an entirely new structural phase wherein oxygen vacancies order in two dimensions.

[1] S.V. Kalinin and N.A. Spaldin, Science 341, 858 (2013)
[2] L. Yao, S. Inkinen, and S. van Dijken, Nature Commun. 8, 14544 (2017)

Controlling defect distribution and intrinsic polarization state ultrathin ferroelectric films

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Understanding and controlling the intrinsic polarization state in ultrathin ferroelectric films is both fundamentally fascinating and crucial for many proposed application of these films, such as potential memory devices, memristors, or a platform for novel integrated electronics using domain wall conduction. This intrinsic polarization results from the interplay of the depolarization field, stemming from the bound charges at the interfaces of the film, which destabilizes the uniform polarization configuration [1,2], and of the built-in field, which favors one polarization direction over the other [3]. The former must be compensated by screening either by external free charges from metallic electrodes or ions from the atmosphere, or by internal mobile charges from within the large-band-gap semiconducting ferroelectric itself to maintain a uniform polarization configuration. The latter results from an asymmetry in this screening or from internal sources, such as trapped charges or charged defect dipole complexes.
We show that we can manipulate both these fields, acting on the electrostatic boundary conditions via the use of dielectric spacer layers to increase the depolarizing field [2,3], or modulating the built-in field and defect distribution through changes in the growth temperature of PbTiO3 thin films, allowing full control over the intrinsic polarization state (monodomain up vs. polydomain vs. monodomain down). We use piezoresponse force microscopy to map the changes in polarization state, while modern Rutherford backscattering spectroscopy allows us to quantify differences in defect density and distribution. We also attempt to measure the depth profile of these defects, both in real space using transmission electron microscopy, and in reciprocal space using X-ray diffraction. Temperature dependent X-ray diffraction measurements complete this dataset, allowing us to track the temperature-dependence of the defect distribution. A Ginzburg-Landau-Devonshire type free energy expansion helps us to tie all our experimental results together.

[1] C. Lichtensteiger et al, Ferroelectricity in ultrathin-film capacitors, Ch. 12 in Oxide Ultrathin Films, Science and Technology, Wiley (2011) (arXiv:1208.5309v1 [cond-mat.mtrl-sci])
[2] C. Lichtensteiger et al, Tuning of the depolarization field and nanodomain structure in ferroelectric thin films, NanoLetters, 14(8), 42025 (2014)
[3] C. Lichtensteiger et al, Built-in voltage in thin ferroelectric PbTiO3 films: the effect of electrostatic boundary conditions, New Journal of Physics, 18, 04 3030 (2016)

$BaHf_{1-x}Ti_xO_3$, high-k perovskite dielectric

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Interest in high-k materials continues as the semiconductor devices shrink in size and in its operating voltage. BaTiO3 is a well-known perovskite ferroelectric material and BaHfO3 is a perovskite high-k dielectric material with a dielectric value of 38. [1] In this study, we fabricated capacitors with an atomically-mixed BaHf1-xTixO3 (BHT, with x varying from 0 to 0.8) layer as the dielectric insulator, and a perovskite semiconductor La-doped BaSnO3(BLSO) layer as the electrode. All the layers were epitaxially grown on SrTiO3 substrates by pulsed laser deposition. X-Ray diffraction was used to investigate the structural properties, from which we confirmed the epitaxial growth of all the layers and obtained their respective lattice constants. The electrical properties of the capacitors, such as the capacitance and breakdown field, were measured. As the x value increased, the relative permittivity value increased and the dielectric breakdown field decreased. We will discuss the alloying level (x value) that maximizes the modulation 2D charge density. Furthermore, we will report on the field effect transistor performances with BHT as the gate dielectric and BLSO as the channel layer to confirm the carrier modulation.

[1] Y. M. Kim et al., "High-k perovskite gate oxide BaHfO3", APL Materials 5, 016104 (2017).

Magnetic and Dielectric Properties of Strained Garnet Ferrite Thin Films

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Rare-earth iron garnet (RIG) is a ferrimagnetic insulator and has a cubic structure with space group Ia3d in bulk. Among various RIGs, $Y_3Fe_5O_{12}$ (YIG) is widely used in ferromagnetic resonance (FMR) and microwave applications as well as studies on spin dynamics since the intrinsic Gilbert damping constant is exceptionally low as $\alpha = 10^{-5}$. YIG grown on $Gd_3Ga_5O_{12}$ (GGG) has shape anisotropy with in-plane easy axis, while YIG on $Y_3Al_5O_{12}$ shows strain-tunable magnetocrystalline anisotropy due to the strain-induced tetragonal distortion [1]. On the other hand, perpendicular magnetic anisotropy is reported in strained $Tm_3Fe_5O_{12}$ (TmIG) [2] and $Sm_3Fe_5O_{12}$ (SmIG) [3] thin films. Epitaxial strain can modify the physical properties such as magnetocrystalline anisotropy and dielectric properties. In this research, magnetic and optical properties of SmIG thin films deposited on GGG substrates are discussed, where lattice strain and relaxation coexist. The lattice mismatch between SmIG and GGG is 1.2%, so that the critical thickness tc, where misfit dislocation occurs, is estimated to be 66 nm. When the thickness of SmIG is thicker than t_c, strain-gradient structure is expected between coherently strained tetragonal and relaxed cubic phases. The strain-gradient structure is directly observed through scanning transmission electron microscope (STEM) analysis. When the thickness of SmIG film is around t_c, large dielectric constant caused by flexoelectricity is observed. Furthermore, the magnetic coercivity increased because defects work as pinning sites of domain wall.

[1] H. Wang et al. Phy Rev B 89 134404 (2014).
[2] C. Tang et al. Phys Rev B 94 140403 (2016).
[3] H. Yamahara et al. J.Mag. Mag. Mater. 323 3143 (2011).

Thermionic Field Emission in back-to-back $BaTiO_3$-based Schottky interfaces

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Ferroelectric tunnel junctions (FTJs) are composed of one thin layer of ferroelectric semiconductor sandwiched by two metallic electrodes. In case of $BaTiO_3$ or other ferroelectric perovskites, to get a full description of the device electric behavior the semiconducting nature of the dielectric and the concomitant formation of Schottky barriers at electrode/ferroelectric interfaces must be explicitly considered. Accordingly, most typically, when M1/$BaTiO_3$/M2 (M1 and M2 are different metallic electrodes) is measured, a rectifying *I(V)* characteristics is recorded. The device architecture corresponds to that of two back-to-back connected Schottky diodes.

In this configuration, one of the diodes is unavoidably reversely polarized and thus the current flowing across it is limited by the corresponding reverse current. Therefore, the current should be limited for any sign of the voltage bias. This is in contrast with some experimental results [1, 2].

On the other hand, bulk $BaTiO_3$ is a n-type semiconductor and thus the BTO/M Schottky diodes is forward biased when $V>0$ is connected to the metal electrode and thus should conduct more for $V>0$ than for $V<0$. In contrast with this expectation, BTO/M junctions are reported to conduct more for $V<0$ [3], raising some doubts either on the nature (n or p) of the BTO films or on the mechanism of transport across the Schottky barrier.

Here, based on the fact that the depletion layer is BTO can be extremely narrow ($\approx$ nm), we build a back-to-back Schottky diode model in which the current across is junctions controlled by Tunnel Field Emission rather than thermal injection. It turns out that in this configuration the reverse current is much enhanced. The model is first successfully tested by computing $I(V)$ data for standard semiconductors and comparing to experimental data. Next, $I(V)$ are collected for Pt (20 nm) / $BaTiO_3$ (5 nm) / $La_{0.67}Sr_{0.33}MnO_3$ (30 nm) capacitors. The model is able to reproduce the observed results for both $V>0$ and $V<0$ biases only if Thermionic Field Emission is included as conduction mechanism. The implications of these findings for understanding $BaTiO_3$-based ferroelectric are discussed.

[1] Nano Lett. 9, 3539-3543 (2009)
[2] Nat. Mater. 11, 860-864 (2012)
[3] Phys. Chem. Chem. Phys. 18, 197-204 (2016)

Non-volatile Ferroelectric Domain Wall Memory

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Ferroelectric domain walls are atomically-sharp topological defects that separate regions of uniform polarization. The discovery of electrical conductivity in specific types of walls gave rise to "domain wall nanoelectronics", a technology in which the wall (rather than the domain) stores information. This paradigm shift critically hinges on precise nano-engineering of reconfigurable domain walls. Here, we demonstrate a prototype non-volatile ferroelectric domain wall memory, scalable to below 100 nm, whose binary state is defined by the existence or absence of conductive walls. The device can be read-out nondestructively at moderate voltages (< 3 V), exhibits relatively high OFF-ON ratios ($\sim 10^3$) with excellent endurance and retention characteristics, and possesses multilevel data storage capacity. This achievement is made possible through a combination of electron beam (e-beam) nanolithography, judicious selection of the crystallographic growth direction of high-quality epitaxial bis- muth ferrite thin films and custom-designed scanning probe microscopy (SPM) approaches. In particular, the specially designed in-plane geometry of the electrodes allows for encoding and retrieval of in- formation via moderate electric fields rather than electric currents, thus enabling low-energy operation. The low-voltage, pulse-based readout of the written states is nondestructive. Furthermore, the re- configurable FEDWs enable a possibility of achieving multilevel data storage; a series of sequentially distinct resistance states can be tuned in a stepwise manner via precise control of DW length. Therefore, data storage densities of these FEDW memory devices can be improved markedly compared to what is achievable using traditional binary bits. Our work thus constitutes an important step toward integrated nanoscale ferroelectric domain wall memory devices.

This work is a collaboration between UNSW Sydney, U Washington, Xiangtan University, St. Louis University and Shenzen Institutes of Advanced Technology.

[1] Sharma et al., Sci. Adv. 2017; 3:e1700512

From local to macroscale switching dynamics in $Pb(Zr_{0.2}Ti_{0.8})O_3$ thin films

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Defects have been shown to greatly impact the intrinsic configuration, geometry and growth of polarization domains in ferroelectric thin films. For example, they can induce different switching dynamics, with polarization reversal dominated either by the nucleation of new domains or by the motion of existing domain walls[1–3]. Defects such as oxygen vacancies can also play an important role in controlling the electrical conduction at ferroelectric domain walls[4] and, in conjunction with electrostatic boundary conditions can even allow fully reversible control of this phenomenon[5]. The local effect of these individual defects or clusters of defects contribute together to the macroscale switching dynamics. Therefore, a bottom-up approach in understanding polarization switching, and making the link between the local and overall behaviour, is crucial.

Here, we present our study of $Pb(Zr_{0.2}Ti_{0.8})O_3$ thin films with different defect landscapes, grown by pulsed laser deposition and radio-frequency magnetron sputtering, which show strikingly different nucleation-dominated vs. domain-wall-motion dominated switching dynamics. Tracking these dynamics over long-duration measurements under both constant and slowly increasing positive and negative bias, using a computer-vision-based distortion correction algorithm[6], we map with 1-2 pixel fidelity the individual domain nucleation, motion and merging events which contribute to the macroscale polarisation switching. While locally "jerky", these individual events lead to an overall average creep-like dynamics. Statistical analysis of the size/power spectrum of the "jerks" resembles the avalanche statistics previously observed in compressed ferroelastics[7], although with unusually large values of the characteristic exponent, possibly linked to inhomogeneous distribution of pinning centers.

[1] Takagi, Ishibashi, Journ. Phys. Soc. Jap. 31, (1971)
[2] Tagantsev et al, PRB 86, 214109 (2002)
[3] Gruverman et al, APL 87, 082902 (2005)
[4] Guyonnet et al, Adv. Mat. 23, 147601 (2012)
[5] Gaponenko et al, APL 106, 162902 (2015)
[6] Gaponenko et al, Sci. Rep. 7, 669 (2017)
[7] Salje, Dahmen, Annu. Rev. Condens. Matter Phys. 5, 233-254 (2014)

Magnetoelectric coupling through the electric-field controlled ionic evolution

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Electric-field control of phase transformation with ion transfer is of great interests in materials science with enormous practical applications. Due to the strongelectron-ion interaction, the ionic evolution would naturally have dramatic influence ont the material magnetic properties. In this talk, I will propose twostrategies/pathways to achieve the magnetoelectric coupling through the electric-field controlled ionic evolution. Firstly, I will present a reversible andnonvolatile electric-field control of oxygen and hydrogen ion evolutions within the model system of brownmillerite $SrCoO_{2.5}$ by ionic liquid gating. Due to theselectively controllable ionic evolutions, we achieved a tri-state phase transformations among $SrCoO_{2.5}$ and its counterpart of perovskite $SrCoO_{3-\delta}$ and ahitherto-unexplored $HSrCoO_{2.5}$ phase. Because of the extremely distinct magnetic, electrical and optical properties among these phases, this result formssolid foundations for the conceptually new tri-state magnetoelectric and electrochromic effects. Next, using $Co/SrCoO_{2.5}$ heterostructure as model system, I will introduce a room temperature electric-field control of magnetic state in the Co layer accompanied by the bipolar resistance switch. In this case, theelectric field controlled oxygen evolution leads to the oxygen ion accumulation (gating) at the interface, in the same manner as the conventional charge gatingdevice. As the consequence, the interfacial oxygen contents modulate the magnetic interaction within the Co surface layer and eventually results inthe intriguing magnetoelectric coupling. We envision that the ionic evolution brings in a new tuning knob to manipulate the coupling and correlation betweencharge, spin, orbital and lattice degrees of freedom and paves a new playground for the discovery of novel materials and rich functionalities.

[1] N. P. Lu, ..., P. Yu*, Nature 546, 124(2017)
[2] H. B. Li, ..., P. Yu*, Nature Communications 8, 2156 (2017)

Electrical and Magnetic Properties of Hexagonal $TbMnO_3$-based Heterostructures

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Rare earth perovskite manganites, $ReMnO_3$, Re=La, Pr, Sm, Tb, Dy, Lu etc generally crystallize in an orthorhombic phase for bigger cationic radii Re=La, Pr, Nd,... They can be artificially stabilized in a hexagonal phase for the rare earth elements with a smaller cationic radius, like Tb, Ho, Dy, Lu. This hexagonal phase is proposed to be a suitable candidate for magneto-electric multiferroics. Here we report the growth of epitaxial hexagonal $TbMnO_3$ thin films on single-crystalline YSZ(111) substrates by means of a metalorganic aerosol deposition (MAD) technique. The XRD patterns reveal that prepared films are fully epitaxial with the (001) plane of the film oriented parallel to the (111) plane of the substrate, i.e. $TbMnO_3$(001)/YSZ(111). Though the orthorhombic phase is well explored, a detailed investigation is needed for the hexagonal phase. Previously, the hexagonal $TbMnO_3$ was reported to be ferroelectric at room temperature with a weak magneto-electric coupling at low temperatures. An electric field control of magnetism in a hexagonal $La_{0.7}Sr_{0.3}MnO_3$/$TbMnO_3$/YSZ(111) hetero-structure will be reported.

[1] T. Kimura, T. Goto, H. Shintani, K. Ishizaka, T. Arima, and Y. Tokura, Nature **426**, 55 (2003)
[2] D.J. Kim, T.R. Paudel, H. Lu, J.D. Burton, J.G. Connell, E.Y. Tsymbal, S.S.A. Seo, and A. Gruverman, Adv. Mater. **26**, 7660 (2014)
[3] J.H. Lee, D. Lee, T.W. Noh, P. Murugavel, J.W. Kim, K.H. Kim, Y. Jo, M.H. Jung, J.G. Yoon, and J.S. Chung, J. Mater. Res. **22**, 2156 (2007)

Flexoelectric polarizations at ferroelastic domain walls in non-ferroelectric WO_3 thin films

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It has been known that WO_3 has a centrosymmetric monoclinic structure at room temperature with a peculiar hierarchicaltwin-domain structure [1]. The twin walls are different from the domain areas in terms of electronic structure and ionic potential, and they are stable places where charged particles such as electrons and point defects gather. In addition, the twin walls where two different ferroelastic domains are colliding provide a unique crystal structure due to the existence of strain gradients, whereby leading to the flexoelectric phenomenon which is a universal physical property existing in all crystalline materials. Experimental observations of polarizations purely caused by the flexoelectric effect, however, are few. In this work, we present emergence of the flexoelectric polarizations at the twin walls in the non-ferroelectric material, which is characterized by angle-resolved piezoresponse force microscope [2].

[1] S. Yun et al., Applied Physics Letters 107, 252904 (2015)
[2] K. Chu et al., Nature Nanotechnology 10, 972 (2015)

Giant polarization sustainability in ultrathin ferroelectric films characterized by Cs-corrected transmission electron microscopy.

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Ferroelectricity is generally deteriorated or even vanished when the ferroelectric films are downsized to unit cell scale, which hampers the potential minimization of ferroelectric-based electronic devices. To maintain and enhance the polarization in nanoscale ferroelectrics is of importance in both scientific and application aspects. Very recently, by tailoring the interface engineering, the polarization in $PbTiO_3$ layer can be greatly increased at $PbTiO_3/BiFeO_3$ bilayers grown on $SrTiO_3$ substrates, which attributes to the oxygen vacancy accumulation at $PbTiO_3/BiFeO_3$ interfaces.[1] In addition, oxygen vacancy is found to play an important role in improving the polarization in $BaTiO_3$ films grown on $SrTiO_3$ substrates as well.[2]

Here we report giant polarization sustainability in a series of ultrathin $PbTiO_3$ films scaled down to several unit cells grown on $NdGaO_3(110)$ substrates with $La_{0.7}Sr_{0.3}MnO_3$ as bottom electrodes. Atomic mappings via aberration-corrected scanning transmission electron microscopy demonstrate the robust ferroelectricity even for the film with the thickness of unit cell scale, as further confirmed by the piezoelectric response in the 3.6nm-thick film. For the 1.2 nm thick film, the calculated polarization reaches 50 μC cm^{-2}. The 2 nm-thick film possesses a polarization as high as the bulk value. The films ranging from 10nm to 35nm thick display a giant out-of-plane lattice parameter, which corresponds to a polarization of 100μC cm^{-2}, 20% larger than that of the bulk $PbTiO_3$. The giant polarization sustainability in the present films is proposed to result from the charge transfer at the $La_{0.7}Sr_{0.3}MnO_3/PbTiO_3$ interface, as supported by the anomalous decrease of Mn valence measured from X-ray photoelectron spectroscopy. This present study reveals the significant role of charge transfer to enhance the large polarization in ultrathin ferroelectrics particularly in the films below 10nm, which will be very helpful for the development of future electronic devices.

[1] Y. Liu, Y.L. Zhu, Y.L. Tang et al., Nano Lett, 17, 3619-3628 (2017).
[2] Q. Qiao, Y. Zhang, R. Contreras-Guerrero, R. Droopad, S. T. Pantelides, S. J. Pennycook, S. Ogut, R. F. Klie, Appl. Phys. Lett. 107, 201604(2015).

Electrostatic control of the band structure and of superconductivity at the $LaAlO_3$-$SrTiO_3$ interface

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The two-dimensional electron system at the interface between $LaAlO_3$ and $SrTiO_3$ has several unique properties that can be tuned by an externally applied gate voltage. The prospect of using these properties in future electronic applications has sparked intensive research efforts over the past decade. However, the fundamental mechanisms underlying this tunability are still not fully understood, as well as the factors that determine the effective band structure at the interface.

In our magnetotransport experiments on topgated Hall bars, the extremely low gate leakage current enables exploration of a larger carrier density range than before. Our data reveal a $d_{xz,yz}$ Lifshitz transition at a carrier density of 2.9 x 10^{13} cm^{-2} and a surprising reduction of dxy-type carrier density with gate voltage above this transition. These observations indicate a gate-tunable band structure, which is controlled by the electrostatic confinement. Self-consistent Schrödinger-Poisson calculations support this conclusion: they reproduce the observed reduction of d_{xy}-type charge carrier density by including interband electronic correlations. [1]

In combination with backgating, we show that the topgated $d_{xz,yz}$ Lifshitz transition can be tuned by a backgate voltage, establishing full electrostatic control of the band structure and confinement of the system. We confirm these experimental results by adding the effect of a backgate voltage to the Schrödinger-Poisson calculations.

As a first step to study the implications of the gate-tunable band structure, we investigated the top- and backgate dependence of the superconducting critical temperature T_c. We observe a distinctly different response to both gate voltages. Subsequent magnetotransport studies above T_c show perfect gate reversibility, enabling a direct comparison of the evolution of T_c with the band filling. This comparison shows that maximum T_c consistently concurs with a kink in tuning the d_{xy} carrier density with gate voltage. Schrödinger-Poisson calculations reproduce this behavior and show that this kink is due to a Lifshitz transition of a second subband of d_{xy} character. This result shows that a full description of superconductivity at $SrTiO_3$-based interfaces must be based on (relative) subband filling, rather than on more conventional parameters like total carrier density or sheet conductivity. [2]

[1] A.E.M. Smink et al. Phys. Rev. Lett. 118, 106401 (2017)
[2] A.E.M. Smink et al. arXiv:1801.02881 (2018)

Hole carriers driving superconductivity in infinite-layer cuprates

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In cuprate superconductors, the infinite-layer (IL) structure is vital for high temperature superconductivity. The fact that the superconductivity in cuprates is always accompanied by competing/coexisting ordering phenomena has puzzled scientists for a long time while investigations into IL cuprates have been hampered by difficulty in preparing high quality samples. In this talk, we show that the evolution of the Hall coefficients (R_{H}) for IL-$Ca_{1-x}RE_xCuO_2$ and IL-$Ca_{1-y}Sr_yCuO_2$ thin films as a function of annealing conditions and film thickness, are crucial parameters for induction of superconductivity. Single crystalline samples of IL cuprates were prepared by reactive molecular beam epitaxy. High resolution x-ray diffraction and high resolution scanning transmission electron microscopy measurements confirmed perfect cation arrangement over the entire film thickness (t = 10-100 nm). Such non-superconducting electron-doped IL-$Ca_{0.916}La_{0.084}CuO_2$ shows electronlike mobile carriers, in contrast to holelike mobile carriers found in superconducting electron doped IL-$Sr_{0.9}La_{0.1}CuO_2$ [1]. Negative R_{H} observed in IL-$Ca_{0.916}La_{0.084}CuO_2$ films can be linked to a formation of electron pockets on the Fermi surface (FS) [2], but their origin of this FS reconstruction requiring long range order parameter, remains unclear. Recent resonant elastic x-ray scattering has revealed charge ordering in IL cuprates [3], and it is a potential candidate for triggering the FS reconstruction. From Hall measurements over 50 IL films we conclude that superconductivity coincides with positive R_{H} and this has also been reported for superconducting $(CaCuO_2)_n/(SrTiO_3)_m$ superlattices [4]. Given the fact that all cuprates are derivative of IL phase, holelike FS seems universal [5,6].

[1] Y. Krockenberger et al., APEX. 7, 063101 (2014).
[2] J.W. Harter et al., Phys. Rev. Lett. 109, 267001 (2012).
[3] H. Wei et al., http://meetings.aps.org/link/BAPS.2017.MAR.K41.7.
[4] D.Di Castro et al., Phys. Rev. B 86, 134524 (2012).
[5] N.P. Breznay et al., Phys. Rev. B 94, 104514 (2016).
[6] S.E. Sebastian et al., Annu. Rev. Condens. Matter Phys. 6, 411 (2015).

Gate tunable carrier density and mobility at the $LaAlO_3/SrTiO_3$ interface

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Pulsed laser deposition is used for almost every study of the two-dimensional electron system (2DES) at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface. Here we show that 90° off-axis magnetron sputtering in Ar yields interfaces with the same quality, where we can investigate subtle details of the electronic behavior similar to what is being done with PLD-grown samples. The Ar-gas pressure also allows precise control over the La/Al ratio x of the films. For films with x <0.97 the films show the well-known metallic behavior. Magneto-transport measurements were performed on back-gated Hall bars at 4.2 K and 1.2 K. In order to properly separate the two conduction subbands the magnetic field was swept between ±15 T. The gate tunability was studied in two doping regimes, moderately-doped (50 V) and heavily-doped (200 V). It revealed that the filling and depletion of the quantum well was quite different in the two regimes. For moderate doping, the carrier density of the high-mobility subband decreases as the gate voltage decreases. However, in the heavily-doped regime, when the gate voltage decreases, the carrier density of the high-mobility subband increases. The carrier density and the low-mobility subband were found to be not sensitive to temperature. However, the high-mobility subband showed an enhanced mobility at lower temperature. We observed a Lifshitz transition at a carrier density of $1.7 \times 10^{13}\,\mathrm{cm}^{-2}$.

Tuning the electronic and magnetic properties of γ-$Al_2O_3/SrTiO_3$

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The many fascinating properties observed in oxide heterostructures have attracted a lot of interest in recent years. Most noticeably, the confined electron gas formed at the interface between the two insulators $LaAlO_3$ and $SrTiO_3$ features, e.g., gate-tunable superconductivity, ferromagnetism and non-volatile memory effects. Numerous studies have been devoted to understand the origin of the conductivity along with enhancing its properties, in particular the electron mobility. Recently, we found[1] that substituting perovskite $LaAlO_3$ with spinel γ-Al_2O_3 can produce a confined electron gas with a record-high electron mobility exceeding 140,000 cm^2/Vs. Here, we show that the γ-$Al_2O_3/SrTiO_3$ interface conductivity originates from oxygen vacancies and use defect engineering to control various interface properties[2–6]. In addition, we reproduce the high mobility and show that it coexists with a strain-tunable magnetic order below 40 K and a positive, non-saturating magnetoresistance of up to 80,000% at 15 T and 2 K. The study points to the γ-$Al_2O_3/SrTiO_3$ heterostructure being an ideal system for exploring the interplay of lattice, spin and electronic degrees of freedom.

[1] Chen YZ, Bovet N, Trier F, Christensen DV et al. A high-mobility two-dimensional electron gas at the spinel/perovskite interface of γ-Al2O3/SrTiO3. Nature Communications (2013), 4:1371.
[2] Christensen DV et al. Controlling the Carrier Density of SrTiO3-based Heterostructures with Annealing. Advanced Electronic Materials (2017), 1700026.
[3] Christensen DV et al. Electron mobility in γ-Al2O3/SrTiO3. Phys Rev Appl. 2018, 9:054004.
[4] Schütz P, Christensen DV et al. Microscopic origin of the mobility enhancement at a spinel/perovskite oxide heterointerface revealed by photoemission spectroscopy. Phys Rev B. 2017, 96:161409.
[5] Gunkel F, Hoffmann-Eifert S, Heinen RA, Christensen DV et al. Thermodynamic Ground States of Complex Oxide Heterointerfaces. ACS Appl Mater Interfaces. 2017, 9:1086.
[6] Christensen DV and Smith A. Is γ-Al2O3 polar? Appl Surf Sci. 2017, 423:887.

Observation of the topological Hall efect in SrRuO3 thin-films.

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Magnetic skyrmions are a topologically protected collection of spins characterized by a chiral structure and are associated with a topological integer which cannot be altered by a continuous deformation of the field configuration. Magnetic skyrmions are expected to be robust under thermal and quantum fluctuations, and are therefore of great interest to material and technological research.

The Dzyloshinskii-Moriya interaction (DMI) plays a role in the formation and stabilization of skyrmions and requires spin-orbit interaction (SOI). Therefore, one would expect to find magnetic skyrmions abundant in 4d and 5d transition metal oxides which exhibit strong SOI. Indeed, magnetic skyrmions have been reported in a few complex-oxide systems such as EuO1-δ [1] and SrRuO3-SrIrO3 [2].

In this presentation, we report that highly-conductive SrRuO3 epitaxial thin-films exhibit the topological Hall effect (THE) across a range of magnetic fields, at low temperatures. The THE is presumably associated with magnetic skyrmions generated in the sample. By measuring the magnitude of the THE and the angle at which the THE vanishes we have estimated the density and size of the magnetic skyrmions. We will discuss possible origins of DMI in this relatively simple system, which enables the formation of magnetic skyrmions.

[1] Y. Ohuchi, et. al. Phys. Rev. B, 91, 245115 (2015).
[2] J. Matsuno, et. al. Sci. Adv. 2, e1600304 (2016).

Angular Photoemission Spectroscopy investigation of STO/YBCO interface.

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Selected complex oxides can be stacked in multi-layer epitaxial heterostructures exhibiting an enhancement or even new properties with respect to the parent compounds. The electronic reconstruction or the strain at interface in these structures is expected to induce modifications of the electrical properties, i.e. changing in the electronic density of state. Here we investigate the electronic properties of $YBa_2Cu_3O_{7-\delta}$ (YBCO) thin film at the interface with $SrTiO_3$ (STO) dielectric insulator. We use soft-X-ray angle-resolved photoelectron spectroscopy (SX-ARPES) to access electronic states at buried of STO/YBCO interface. We studied for the first time by SX-ARPES the Fermi surface of YBCO thin film and its modification due to the introduction of STO/YBCO interface. Complementary investigations by means of resonant photo-emission spectroscopy across the Ti L2,3 absorption edge were performed to study electronic states of the insulating STO near the YBCO interface.

Cation substitution driven apical oxygen vacancies in overdoped La-214 cuprates and its superconducting properties

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In the high temperature superconductors the superconducting properties are functions of carrier concentration, which is controlled by the concentration of defects including heterovalent cations, interstitial oxygen ions, and oxygen vacancies [1]. These three kinds of dopants are all closely interrelated in the growth process according to the defect chemistry [2]. Here we combine low temperature thermal treatment of $La_{2-x}Sr_xCuO_4$ (LSCO) epitaxial thin films grown by oxide molecular beam epitaxy and polarized Raman spectroscopy to control and investigate oxygen vacancies. We demonstrate that the apical site is the most favorable position to accommodate oxygen vacancies under low temperature annealing. Additionally we investigate the superconducting properties of heavily overdoped La-214 thin films, which shows different phase diagram from that of bulk, and demonstrate that the concentration of oxygen vacancies increases deforming the oxygen network as the dopant concentration increases. This observation is consistent with previous defect chemistry studies [2], and calls for further investigation of the defect induced properties in the overdoped regime of the hole-doped lanthanum cuprates [3, 4].

[1] B. Keimer, et al., Nature 518, 179 (2015)
[2] J. Maier and G. Pfeundtner, Adv. Mater. 3, 292 (1991)
[3] Božović, et al., Nature 536, 309 (2016)
[4] N. R. Lee-Hone, et al., arXiv:1704.04803 (2017)

Unveiling the superconducting mechanism of $Ba_{0.51}K_{0.49}BiO_3$

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Bismuthates were the first family of oxide high-temperature superconductors [1], exhibiting superconducting transition temperatures (Tc) up to 32 K (Refs. 2 and 3), but the superconducting mechanism remains under debate despite more than 30 years of extensive research. Our angle-resolved photoemission spectroscopy studies on $Ba_{0:51}K_{0:49}BiO_3$ reveal an unexpectedly 34% larger bandwidth than in conventional density functional theory calculations. This can be reproduced by calculations that fully account for long-range Coulomb interactions - the first direct demonstration of bandwidth expansion due to the Fock exchange term, a long-accepted and yet uncorroborated fundamental effect in many body physics [4]. Furthermore, we observe an isotropic superconducting gap with $2\Delta_0 = k_B T_c = 3.51 \pm 0.05$, and strong electron-phonon interactions with a coupling constant $\lambda \sim 1.3 \pm 0.2$. These findings solve a long-standing mystery - $Ba_{0.51}K_{0.49}BiO_3$ is an extraordinary Bardeen-Cooper-Schrieffer (BCS) superconductor, where long-range Coulomb interactions expand the bandwidth, enhance electron-phonon coupling, and generate the high Tc. Such effects will also be critical for finding new superconductors.

[1] A. W. Sleight, J. L. Gillson, and P. E. Bierstedt, Solid State Communications 17, 27 (1975).
[2] L. F. Mattheiss, E. M. Gyorgy, and D. W. Johnson, Physical Review B 37, 3745 (1988)
[3] R. J. Cava, B. Batlogg, J. J. Krajewski, R. Farrow, L. W. Rupp, A. E. White, K. Short, W. F. Peck, and T. Kometani, Nature 332, 814 (1988).
[4] N.W. Ashcroft and N. D. Mermin, "Solid State Physics," (Holt, Rinehart and Winston, 1976) Chap. 17, pp. 334-337.

Magnetotransport at $SrTiO_3/LaTiO_3$ interfaces

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In recent years, there has been considerable interest in oxide heterostructures due to possible new applications in nanoscale electronics. In particular, the $LaAlO_3/SrTiO_3$ interface has been studied in detail due to possible switching or spintronic device applications[1]. A two-dimensional electron gas in a strongly asymmetric quantum well has been observed at this interface, but it has proven to be difficult to analyze the carrier density in the electron gas because several mechanisms, including polar discontinuity, interdiffusion, and lattice defects may contribute.

For this work, we have chosen to use a similar electronic system of $LaTiO_3/SrTiO_3$, where the main advantage is that the total carrier number in the system can be adjusted over a wide range by changing the number of La atoms in the $LaTiO_3$ doping layer in $SrTiO_3$. Due to the variable valence of Ti, polarity effects should be minimal in this system. Our main interest is to study how electrons respond to an external magnetic field and to attempt to determine if a magnetically ordered state exists at this interface.

The heterostructures were grown by pulsed laser deposition, embedding $LaTiO_3$ layers in $SrTiO_3$. Similar to the earlier work on $LaAlO_3/SrTiO_3$ interfaces[2], a large negative in-plane magnetoresistance effect occurs in this heterostructures at low temperature when the magnetic field is applied parallel to the current. Additionally, it is observed in transport measurements that not all carriers are confined to the quantum well but may be distributed over a larger distance from the interface in the $SrTiO_3$ substrate.

We also discuss back-gated magnetotransport measurement data where the carrier depth distribution in the heterostructure is tuned and attempt to distinguish which carriers are responsible for the observed negative in-plane parallel magnetoresistance.

[1] N. Reyren, M. Bibes, E. Lesne, J.-M. George, C. Deranlot, S. Collin, A. Barthelemy, and H. Jaffres, Phys. Rev. Lett. **108**, 186802 (2012)
[2] M. Diez, A. M. R. V. L. Monteiro, G. Mattoni, E. Cobanera, T. Hyart, E. Mulazimoglu, N. Bovenzi, C. W. J. Beenakker, and A. D. Caviglia, Phs. Rev. Lett. **115**, 016803 (2015)

Examination of synergetic conductance in graphene-$SrTiO_3$ thin film heterostructure

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Synergetic effects on heterostructures of 2D van der Waals materials and transition metal oxides (TMO) have enthusiastically researched. Despite their potential as multifunctional devices, it has been quite tough to achieve high-quality of both graphene and $SrTiO_3$ (STO) thin film, preventing from investigating the combined phenomena such as quantum Hall hysteresis. In this work, we successfully observed the magnetoconductance behavior of monolayer graphene on epitaxial STO single-crystalline thin film. High dielectric constant nature of STO thin film leads to the much narrower range of operating voltage than that on a silicon-based substrates [1]. Additionally, large electric field generates/redistributes oxygen vacancies in the STO layer, resulting in a systematic development of hysteresis of conductance on top of quantum Hall nature [2]. By defining the layered capacitor model including the oxygen vacancy accumulation, we have figured out the quantitative relationship among the dielectric properties of STO with oxygen vacancies during the hysteretic transport measurements.

[1] Park, J. et al., Nano Lett. 16, 1754 (2016).
[2] K. T. Kang. et al., Adv. Mater. 29, 1700071 (2017).

Enhancement of Upper Critical Field in Superconducting Sr_2RuO_4 Thin Films

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Growth of superconducting Sr_2RuO_4 thin films has been extremely challenging over the past 25 years [1], since the superconductivity emerges only in crystals with high purity, high crystallinity, and high stoichiometry. Recently we have established molecular beam epitaxy of superconducting Sr_2RuO_4 films by refining electron-beam evaporation techniques [2]. The reproducible growth of superconducting films opens up a new route to study the exotic superconductivity of this compound.
Here we report on superconducting state realized in thin films, which were characterized by measuring angular and temperature dependence of the upper critical field with a dilution refrigerator. Out-of-plane angular dependence is rather well fitted by the Tinkham model, indicating an approach to ideal two-dimensional behavior. With this change, dramatic enhancement of the upper critical field is observed in comparison to the bulk ones, which gives important hints to narrow down possible superconductivity symmetries. Fabrication and characterization of Sr_2RuO_4 Josephson junctions will be also discussed.

[1] Y. Krockenberger, M. Uchida et al., Appl. Phys. Lett. 97, 082502 (2010).
[2] M. Uchida et al., APL Mater. 5, 106108 (2017).

Electronic transport in low dimensions: conducting nanowires at the $LaAlO_3/SrTiO_3$ interface

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At the interface between $LaAlO_3$ and $SrTiO_3$ is confined a two dimensional electron system characterized by several interesting properties. It has a strong Rashba spin-orbit coupling, it is superconducting below 300 mK and its properties can be tuned by an external electric field.
We are currently investigating the effect of in-plane confinement on its electronic properties in order to reveal possible effects of the complex oxide physics in mesoscopic devices.
We present here a detailed study of the electronic magneto-transport in channels characterized by lateral sizes ranging from 1 μm down to 50 nm. The larger structures have been realized by using photo and electron beam lithography whereas the smaller ones have been realized with the AFM-writing technique [1],[2].
Since the size of these devices is close to the typical scattering lengths of the $LaAlO_3/SrTiO_3$ interface we expect to observe deviations from the behavior of standard 2D conducting channels.

[1] Cen, C. et al., Nat Mater 7, 298-302 (2008)
[2] Boselli, M. et al. , Applied Physics Letters 108, 061604 (2016)

Presence of a hole band at the $LaTiO_3/SrTiO_3$ interface

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It is well known that the two-dimensional electronic conductance at the interface between the band insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) derives from Ti d-electron band formation on the TiO_2 side of the interface. However, there are also reports on complementary hole conductance in the LAO layer. In particular, it has been shown that by growth of an STO capping layer on LAO/STO it is possible to create mobile hole gas [1,2]. Here we investigate another oxide interface, between the Mott insulator $LaTiO_3$ (LTO) and STO. We find that the magnetotransport properties exhibit anomalous behaviour in a certain gate range. This behaviour cannot be simply explained by a two-band model based on two electron types of carriers, but that a hole band is present even in these uncapped samples. Carrier concertation of holes are lower than carrier concentration of electrons by a few orders of magnitude. Nevertheless, hole mobility is higher than electron mobility in the gate range corresponding to the anomaly. Stoichiometric LTO is a Mott insulator. However, holes can be introduced into the LTO layer by a small amount of Sr doping [3] and/or a small measure of off-stoichiometry [4]. Furthermore, we have observed that this anomaly of magnetotransport properties correspond to the maximum of the superconducting dome as determined both from sheet resistance and critical current measurements.

[1] Pentcheva, R. et al. Parallel electron-hole bilayer conductivity from electronic interface reconstruction. *Phys. Rev. Lett.* **104**, 166804 (2010).

[2] Lee, H. et al. Direct observation of a two-dimensional hole gas at oxide interfaces. *Nat. Mater.* **17**, 231-236 (2018).

[3] Hays, C. C. et al. Electronic transition in $La_{1-x}Sr_xTiO_3$ *Phys. Rev. B* **60**, 10367 (1999).

[4] Gariglio, S. et al. Transport properties in doped Mott insulator epitaxial $La_{1-y}TiO_{3+\delta}$ thin films. *Phys. Rev. B* **63**, 161103(R) (2001).

Magnetic and electrical properties of combined $LaAlO_3$ and $LaMnO_3$ heterostructures on $SrTiO_3$

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Recent years have seen a surge of scientific interest in perovskite oxides. Due to the large range of interesting and unconventional properties, as well as the ability to be grown epitaxially with ease, thin film perovskites provide a new possible platform for future technologies.
The discovery of the conducting 2-dimensional electron system at the interface of SrTiO3 and LaAlO3, and its associated critical thickness behavior [1], shows that small changes in parameter space can have drastic effects. A similar effect was found in LaMnO3, where above a critical thickness of 6 unit cells, the material spontaneously turns ferromagnetic [2].
One of the leading hypotheses to explain the critical thickness behavior is related to the polar nature of LaAlO3 and LaMnO3. The polar mismatch with the non-polar SrTiO3 substrate causes an internal potential, which is resolved by transfer of electrons towards the interface, causing the abrupt change in properties.
To investigate further into this hypothesis, we have fabricated combined LaAlO3 and LaMnO3 heterostructures on SrTiO3 in various configurations. We explore the influence of two polar layers on the properties of the two component systems. Using a variety of measurement techniques, including Scanning SQUID Microscopy and several synchrotron-based X-ray techniques, we investigate the magnetic and electrical properties of the heterostructures.

[1] S. Thiel et al., Science 313, 2006
[2] X.R. Wang et al., Science 349, 2015

Non 1/B-periodic Shubnikov-de Haas oscillations in gate tunable 2DEG at the $LaAlO_3/SrTiO_3$ interface

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The formation of a two-dimensional electron gas (2DEG) at the interface between two insulators $SrTiO_3$ (STO) and $LaAlO_3$ (LAO) is among the most intriguing finding in oxide electronics. In recent years, several exotic phenomena including superconductivity [1], Rashba spin-orbit coupling [2], ferromagnetism and quantum oscillations [3] have been reported at this interface. While the theoretical calculations for band structure reveal the occupancy of several subbands (d_{xy}, d_{xz} and d_{yz}) arising from the interface crystal field splitting of Ti:3d t_{2g} orbital, no clear consensus has been reached yet from experimental evidences. Here, we investigate the quantum transport of a high mobility 2DEG at LAO/STO interface under high magnetic field (55 T). The Shubnikov-de Haas oscillations (SdHO) in longitudinal resistance (R_{xx}) show a clear monotonic dependence with varying the gate voltage/carrier density, despite a discrepancy between the carrier concentrations estimated from Hall resistance and SdHO frequency. The evolution of the carrier density and electronic mobility with varying back-gate voltage is consistent with charge trapping/de-trapping by defects in STO [4]. Interestingly, the Landau fan diagram is non-linear over the full magnetic field range. We investigate on this phenomenon, which can be either the signature of a magnetic field-driven Lifshitz transition or originates from a complex set of populated sub-bands at the Fermi energy.

[1] A. Joshua et al., Nature Comm. 3, 1129 (2012); J. Biscaras et al., Phys. Rev. Lett. 108, 247004 (2012).
[2] A. D. Caviglia et al., Phys. Rev. Lett. 104, 126803 (2010); Z. Zhong et al., Phys. Rev. B 87, 161102(R) (2013).
[3] B. Shalom et al., Phys. Rev. Lett. 105, 206401 (2010); M. Yang et al., App. Phys. Lett. 109, 122106 (2016).
[4] J. Biscaras et al., Sci. Rep. 4, 6788 (2014).

Layer-Resolved Band Bending at the n-$SrTiO_3(001)$/p-Ge(001) Interface

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The epitaxial n-STO/p-Ge(001) interface shows considerable promise for harvesting visible sunlight to drive the hydrogen evolution reaction (HER) associated with water splitting [1]. The Ge band gap is small (0.66 eV) and band alignment with STO is favorable for electron-hole pair creation and separation [2]. Moreover, the conduction band minimum of STO is above the HER half-cell potential, allowing for energetically favorable electron transfer across the heterojunction/liquid interface and coupling to the HER. In determining the band alignment for n-STO/p-Ge by XPS, we have previously noted a curious broadening in the Ge $3d$ core-level line shape relative to that for pure, clean p-Ge(001)-(2x1) [2]. In principle, such broadening could come from a chemically shifted feature resulting from an interface formation product, or from the presence of a built-in potential within the Ge. Data taken on heterostructures with thinner ($< \sim$10 u.c.) STO films using Al Kα X-rays (1.5 keV) are inconclusive. However, spectra measured on thicker STO/Ge heterojunctions with 6 keV X-rays, along with scanning transmission electron microscopy (STEM) imaging, allow the interface chemical shift explanation to be ruled out. Rather, these data are best explained by band bending in the Ge that spans the entire band gap. We have developed an algorithm that fits the Ge $3d$ spectrum to a linear combination based on a model function describing the spectrum for flat-band p-Ge and yields a potential energy profile for the Ge. The Ge $3d$ binding energy for the interfacial layer is markedly higher than that for layers deeper into the substrate, consistent with the interface structure determined by STEM imaging and first-principles modeling. The conduction band minimum at the interface is degenerate with the Fermi level. The depletion width is $\sim$4 nm wide and the valence band maximum at the bottom is degenerate with the Fermi level. This method allows characteristics of built-in potentials at buried interfaces to be probed in a unique and powerful way, and should be useful for other complex oxide heterostructures as well.

[1] K. A. Stoerzinger, Y. Du, S. R. Spurgeon, L. Wang, D. Kepaptsoglou, Q. M. Ramasse, E. J. Crumlin, S. A. Chambers, MRS Comm. (doi:10.1557/mrc.2018.38).

[2] S. A. Chambers, Y. Comes, S. R. Spurgeon, P. V. Sushko, Appl. Phys. Lett. **110**, 082104 (2017).

Searching for high-mobility two-dimensional electron gas at oxide interfaces through electrolyte gating

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Construction of high-mobility oxide interfaces and modulation of the conductivity are essential for exploration of quantum phenomena and potential application. We demonstrate the modulation of electrical transport properties in both crystalline and amorphous LaAlO3/SrTiO3 (LAO/STO) interfaces by electrolyte gating using electric double layer transistor (EDLT) configuration. For the crystalline LAO/STO interfaces, monotonic tuning of electron mobility and quantum magnetoresistance oscillations over a carrier density range up to one order of magnitude are obtained due to the electrolyte gating induced depletion of charge carrier. For the amorphous LAO/STO (a-LAO/STO) interfaces in which the conductivity is caused by oxygen vacancy formation, it is found that filling of oxygen vacancies and therefore, the decrease in carrier density after liquid gating, suggesting the presence of oxygen migration. The filling effect caused the reconstruction of interfacial band structures, which could be controlled by the LAO overlayer deposition temperature, suggesting a method to tune band structures and oxidation states on buried oxides. Moreover, enhanced carrier mobility of 3,580 cm2/Vs at 3 K and quantum oscillations at a-LAO/STO are achieved as a result of gating-induced oxygen filling. Moreover, electrolyte gating is also performed at the 5d-electron oxide KTaO3-based amorphous interfaces which possesses less effective electron mass and low-temperature mobility higher than 20,000 cm2/Vs is obtained at the interface grown at room temperature.

Spin Hall magnetoresistance in antiferromagnet/heavy-metal heterostructures

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Spintronic devices integrating ferromagnetic materials and heavy metals in multilayer hybrid structures represent well-established basic elements in the field of data storage. For future spintronic applications, antiferromagnetic materials have come into the focus of interest. They promise robustness against external magnetic-field perturbations as well as faster magnetization dynamics compared to simple ferromagnets, paving the way to ultrafast information processing. For the integration of such materials in data storage devices, however, a robust detection scheme for their antiferromagnetic magnetization state is required. The spin Hall magnetoresistance (SMR) could serve as a sensitive probe in this regard [1,2]. Moreover, the SMR only requires a simple planar metallic electrode on top of the antiferromagnet, making it a promising tool for future applications.

We investigate the spin Hall magnetoresistance in thin-film bilayer heterostructures of the heavy metal Pt and the antiferromagnetic insulator NiO [3]. While rotating an external magnetic field in the easy plane of NiO, we record the longitudinal and the transverse resistivity of the Pt layer and observe an amplitude modulation consistent with the spin Hall magnetoresistance. In comparison to Pt on collinear ferrimagnets, the modulation is phase shifted by 90° and its amplitude strongly increases with the magnitude of the magnetic field. We explain the observed magnetic field dependence of the spin Hall magnetoresistance in a comprehensive model taking into account magnetic-field-induced modifications of the domain structure in antiferromagnets. With this generic model, we are further able to estimate the strength of the magnetoelastic coupling in antiferromagnets.

Our detailed study shows that the spin Hall magnetoresistance is a versatile tool to investigate the magnetic spin structure as well as magnetoelastic effects, even in antiferromagnetic multidomain materials.

[1] H. Nakayama et al., Phys. Rev. Lett. 110, 206601 (2013).
[2] M. Althammer et al., Phys. Rev. B 87, 224401 (2013).
[3] J. Fischer et al., Phys. Rev. B 97, 014417 (2018).

Interfacial anomalous Hall effects in ultrathin $LaAlO_3/SrRuO_3$ heterostructures

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Due to a sensitive balance among competing energy scales, oxide interfaces play host to a wide variety of intriguing phenomena absent in their bulk constituents. A material that is currently being considered in the context of geometric phases is $SrRuO_3$ (SRO)[1,2], a 4d itinerant ferromagnet exhibiting an anomalous Hall effect that is directly proportional to the Berry curvature of the occupied bands at the Fermi level [3]. Since the Berry curvature is highly sensitive to small reconstructions of the band structure, oxide interfaces provide a suitable platform for its manipulation[4]. In this work, we study the electronic and magnetic properties of $SrTiO_3/SrRuO_3/LaAlO_3$ (STO/SRO/LAO) heterostructures. We demonstrate the emergence of two opposing anomalous Hall effects originating from different band reconstructions at the STO/SRO and SRO/LAO interfaces. The observed phenomenon is present over a wide (80 K) temperature range and is found to depend critically on the SRO layer thickness. We identify and discuss possible mechanisms. The results underline the potential of manipulation of geometric phases at oxide interfaces and provide new avenues for controlling spin-polarized transport at the nanoscale.

[1] Matsuno, Jobu, et al. "Interface-driven topological Hall effect in SrRuO3-SrIrO3 bilayer." Science advances 2.7 (2016): e1600304.
[2] Ohuchi, Yuki, et al. "Electric-field control of anomalous and topological Hall effects in oxide bilayer thin films." Nature communications 9.1 (2018): 213.
[3] Fang, Zhong, et al. "The anomalous Hall effect and magnetic monopoles in momentum space." Science 302.5642 (2003): 92-95.
[4] Nagaosa, Naoto, et al. "Anomalous hall effect." Reviews of modern physics 82.2 (2010): 1539.

Determination of Spin-Orbit Scattering Lifetime at the Interface of $LaAlO_3/SrTiO_3$ from the Superconducting Upper Critical Fields

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The intrinsic mechanism of the spin-orbit coupling at the $LaAlO_3$ / $SrTiO_3$ interface remains a debatable issue. Rashba-type spin-orbit coupling is an appealing candidate that has been demonstrated by several magnetotransport results. On the other hand, the atomic spin-orbit coupling was also shown to play an important role, particularly when the Fermi level is close to the Liftshitz point. Unlike previous works, we focus on the measurements of the anisotropic and superconducting upper critical fields in gated $LaAlO_3$ / $SrTiO_3$ devices. By rigorous fittings of the H_{c2}-T curves using both the Werthamer-Helfand-Hohenberg theory and Klemm-Luther-Beasley model, the spin-orbit scattering lifetime can be determined with high precision in superconducting state. We found that the extracted spin-orbit lifetime monotonically increase with the transport lifetime that spanned over two orders of magnitude in the regime with sheet density higher than that at Liftshitz point. Those results suggest the dominant role of Elliott-Yafet type spin-relaxation.

Electron Mobility Optimization in High-Pressure-Oxygen-Sputtered Epitaxial $Ba_{1x}La_xSnO_3$ Thin Films

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Among perovskite oxides, the wide gap semiconductor $BaSnO_3$ possesses a uniquely high room temperature electron mobility, making it of great interest for oxide electronics. However, high defect densities limit mobility in $BaSnO_3$ thin films, and, despite recent progress, many questions remain regarding transport behavior and the nature of defects in $BaSnO_3$. Due to a lack of lattice-matched substrates for growth of $BaSnO_3$, the relationship between dislocation density and substrate mismatch is of particular interest. Here, following our prior work with oxygen vacancy doping [1,2], epitaxial films of La-doped BaSnO3 ($Ba_{1x}La_xSnO_3$) have been grown via high-pressure oxygen sputtering on several perovskite substrates spanning a wide range in mismatch (-2.2% to -8.7%), while varying deposition temperature, film thickness, and deposition rate [3]. 300 K mobilities as high as $70\,cm^2V^{-1}s^{-1}$ are achieved at 2 x $10^{20}\,cm^{-3}$ electron densities; these are record values for sputter deposition, comparable to previous reports by PLD. Notable trends include a monotonic increase in mobility with deposition temperature, carrier compensation and reduced mobility at low thickness, optimal thickness that varies with growth rate, and a remarkable insensitivity to lattice mismatch. These findings are discussed in terms of detailed structural characterization, primarily by high-resolution X-ray diffraction and transmission electron microscopy [4,5]. Of particular interest, threading dislocation densities are found to be essentially independent of misfit dislocations densities, explaining the insensitivity of mobility to lattice mismatch in relaxed films [3].

[1] Ganguly, Ambwani, Xu, Jeong, Mkhoyan, Leighton and Jalan, APL Mater. 3, 062509 (2015).
[2] Ganguly, Prakash, Jalan and Leighton, APL Mater. 5, 056102 (2017).
[3] Postiglione, Ganguly, Yun, Jeong, Mkhoyan, Jalan and Leighton, in preparation.
[4] Yun, Topsakal, Prakash, Ganguly, Leighton, Jalan, Wentzcovitch, Mkhoyan and Jeong, J. Vac. Sci. Technol. A 36, 031503 (2018).
[5] Yun, Ganguly, Postiglione, Jalan, Leighton, Mkhoyan and Jeong, in press, Sci. Rep. (2018).

Tuning the Ground State of Oxide Interfaces by an Electron Sink

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The two-dimensional electron liquid (2DEL) formed at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface is related to the electrons located in $3d$-orbit of Ti. Due to electron-electron interactions, the ground state of the system, which is either superconducting or magnetic, is sensitive to the external electric field that changes the carrier density by tuning the shape and width of the potential well [1]. On the other hand, a charge-transfer-induced modulation doping can be made by inserting a $LaMnO_3$(LMO) buffer layer into LAO/STO interface which not only significantly suppresses the carrier density but also boosts the mobility of these carriers[2]. Herein, we report unforeseen tunability of the phase diagram of the metallic LAO/STO interface by introducing an electron sink of ferromagnetic LaMnO3 insulator into the LAO side. This is done without formation of lattice disorder and without changing the polarity of the system, $LaAl_{1-x}Mn_xO_3$/STO ($0 \leq x \leq 1$). By deliberately increasing the Mn-doping level, x, the interfacial 2DEL undergoes a Lifshitz transition [3] at x=0.225 with a critical carrier density of $n_c = 2.8 \times 10^{13}$ cm^{-2}, where a peak value of 250 mK of superconducting transition temperature is observed. Moreover, the $LaAl_{1-x}Mn_xO_3$ turns ferromagnetic at $x \geq 0.25$. Remarkably, at a doping level of x=0.3, before the metallic interface becomes insulating, we observed signatures of both ferromagnetism and superconductivity in the same 2DEL where the d_{xy} electrons are dominated.

[1] A. E. M. Smink, J. C. de Boer, M. P. Stehno, A. Brinkman, W. G. van der Wiel and H. Hilgenkamp, Gate-Tunable Band Structure of the LaAlO3-SrTiO3 Interface, PRL. 118 (2017) 106401. DOI: 10.1103/PhysRevLett.118.106401

[2] Y. Z. Chen et al. Extreme mobility enhancement of two dimensional electron gases at oxide interfaces by charge-transfer-induced modulation doping, Nature Mater. (2015) 14, 801-806. DOI: 10.1038/NMAT4303

[3] Arjun Joshua, S. Pecker, J. Ruhman, E. Altman and S. Ilani, A universal critical density underlying the physics of electrons at the LaAlO3/SrTiO3 interface. Nat. Commun. (2012) 3:1129. DOI: 10.1038/ncomms2116.

2D-like $LaInO_3$ /$BaSnO_3$ polar interface on MgO substrate

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We investigated the $LaInO_3$ (LIO)/La-doped $BaSnO_3$ (BLSO) interface on non-perovskite MgO substrates. LIO/BLSO interface shows two dimensional electron gas(2DEG)-like behavior with conductance enhancement of several orders of magnitude after growth of LIO layer on BLSO layer on MgO substrate. We first confirmed the LIO/BLSO interface structure on MgO substrates. Reciprocal Space Mapping result and Transmission Electron Microscopy image show well-formed LIO/BLSO interface. And we measured electrical properties to see the 2D-like conducting interface. There was clear conductance enhancement after growth of LIO layer on the BLSO layer. This result is similar with the result of LIO/BLSO interface on STO substrate from our previous report [1]. However, we observed large conductance enhancement even at LIO/BSO(undoped) interface in the case on MgO substrate. Using this 2DEG-like interface with undoped BSO on MgO substrates, we fabricated field effect devices. The device shows improved performances when compared with previous devices based on BSO material.

[1] U. Kim et al., APL Materials 4, 071102 (2016).

Dimensionality Effects on the Metal-Insulator Transition in Nickelate Heterostructures

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We propose a theoretical model explaining the insulating behavior of a class of nickelate heterostructures that has recently been studied experimentally (NdNiO3/NdAlO3) [1], based on results from density functional theory and low-energy dynamical mean field theory calculations[2].Our DFT+DMFT calculations find that the reduced dimensionality widens the range of interaction parameters (U,J) for which the material is insulating at a given temperature. Our results suggest that a spontaneously electronically disproportionated, insulating state does not necessarily have to be preceded by a structural disproportionation in the heterostructured material. Further, we find that layer confinement leads to a significant increase in the metal-insulator transition temperature as compared to the bulk material. Finally, electronic disproportionation in the heterostructures leads to a modified pattern of structural disproportionation in the ground state as compared with the bulk, accompanied by structural distortions in the adjacent NdAlO3 layers.These results are likely of a general nature and can be used to understand similar results in the nickelate heterostructure literature as well as in the design of future heterostructures.

[1] 'Control of hidden ground-state order in NdNiO3 superlattices', PRM 1, 024410, 2017
[2] 'Low-energy description of the metal-insulator transition in the rare-earth nickelates', PRB 91, 075128, 2015

First-principles study of $(Ba,Ca)TiO_3$ and $Ba(Ti,Zr)O_3$ solid solutions

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High-performance piezoelectrics are key components of various smart devices and, recently, it has been discovered that $(Ba,Ca)(Ti,Zr)O_3$ (BCTZ) solid solutions show large electromechanical response [1,2,3,4]. Nevertheless, the microscopic origin of such feature is still unclear and theoretical characterizations of BCTZ remain very limited [5, 6]. Accordingly, we present here a first-principles study of the structural and dynamical properties of different compositions of $(Ba,Ca)(Ti,Zr)O_3$ solid solutions and related parent compounds in order to identify the microscopic mechanisms tuning the ferroelectric properties of the system. Specifically, we focus on the distinct effects arising from the Ca and Zr doping in the $(Ba,Ca)TiO_3$ and $Ba(Ti,Zr)O_3$ parent binary-systems, respectively [7].
When going from $BaTiO_3$ to $CaTiO_3$ in $(Ba,Ca)TiO_3$, the main feature is a gradual transformation from *B*-site to *A*-site ferroelectricity due to steric effects that largely determines the behavior of the system. In particular, for low Ca-concentration we found out an overall weakened *B*-driven ferroelectricity that produces the vanishing of the energy barrier between different polar states and results in an isotropic polarization. A sizable enhancement of the piezoelectric response results from this landscape.
When going from $BaTiO_3$ to $BaZrO_3$ in $Ba(Ti,Zr)O_3$, in contrast, the behavior is dominated by cooperative Zr-Ti motions and the local electrostatics. In particular, low Zr-doping produces the further stabilization of the *R3m*-phase. Then, the system shows the tendency to globally reduce the polar distortion with increasing Zr-doping. Nevertheless, ferroelectricity can be locally preserved in Ti-rich regions. Moreover, we also found out an unexpected polar activation of Zr as a function of specific atomic ordering explained via a basic electrostatic model based on $BaZrO_3$ /$m$$BaTiO_3$ superlattice.
Therefore, the mixing of $(Ba,Ca)TiO_3$ and $Ba(Ti,Zr)O_3$ with low concentration of Ca and Zr, like in the interesting composition-range of BCTZ, seems to allow the system to experience different polar states with different polarization orientation separated by low energy barrier. Further investigations are in progress to verify the effect of such energy landscape on the piezoelectric response.

[1] W. Liu and X. Ren, Phys. Rev. Lett., 103, 257602 (2009)
[2] D. S. Keeble et al., Appl. Phys. Lett. 102, 092903 (2013)
[3] M. Acosta et al., Phys. Rev. B, 91, 104108 (2015)
[4] K. Brajesh, M. Abebe, R. Ranjan, Phys. Rev. B, 94, 104108 (2016)
[5] D. Fu and M. Itoh, arXiv:1503.00406 [cond-mat.mtrl-sci] (2015)
[6] Y. Nahas et al., Nat. Commun., 8, 15944 (2017)
[7] D. Amoroso, A. Cano and Ph. Ghosez, arXiv:1801.08886 [cond-mat.mtrl-sci] (2018)

Topological phases of (111) oriented $LaAlO_3$-$SrTiO_3$ interfaces

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Two-dimenional electron fluids (2DES) have been uncovered at surfaces and interfaces of several transition metal oxide perovskites. These 2DES are endowed with properties which are usually not present in the host material(s). In this respect, the LaAlO3-SrTiO3 (LAO-STO) heterostructure is a paradigmatic compound which exhibits metallicity, superconductivity, spin textures stemming from a Rashba spin-orbit contribution, possibly spin fluctuations as well. These properties are tunable with a gate voltage paving the way for technological applications.
In the case of bare surfaces, the existence of the 2DES has been linked to the presence of oxygen vacancies whicht are confined near the boundary. For (001) oriented STO, we recently predicted that the metallic state is in fact a topological phase which should give rise to one-dimensional edge states. The multi-orbital character of the conduction band electrons compounded with confinement and bulk spin-orbit was instrumental in promoting a band inversion leading to the topological regime. A similar scenario is expected for (001) LAO-STO
Here, we turn to the case of (111) oriented LAO-STO where signatures of a 2DES have been found in transport. For this particular orientation, confinement impacts all orbitals equally and one does not expect the same type of crossing points in the Brillouin zone (BZ) that were found for the (001) orientation. Remarkably, we predict two topological regimes in the (111) case. One is linked to a parity inversion at the M points of the honeycomb BZ. This is similar to what we found for (111) STO and KTaO3. We uncover a second topological regime coexisting with the previous one. In the presence of Coulomb interactions, an inversion in the ordering of the sub-bands caused by confinement takes place. This inversion is evidenced in Hall effect measurements. This inversion leads to three-band crossings and in the presence of spin-orbit interactions gives rise to a Z2 topological state, with its own set of edge states. Our findings are based on a tight-binding modeling of the band structure derived from transport and from ARPES (in analogy with STO111) as well as Poisson-Schroedinger calculations including Coulomb effects.

Appearance and disappearance of ferromagnetism in ultra-thin $LaMnO_3$on $SrTiO_3$substrate: a viewpoint from first-principles

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The intrinsic magnetic state (ferromagnetic or antiferromagnetic) of ultrathin $LaMnO_3$ films on the most commonly used $SrTiO_3$ substrate is a long-existing question under debate. Either strain effect or nonstoichiometry was argued to be responsible for the experimental ferromagnetism. In a recent experiment [1], one more mechanism, namely, the self-doping due to polar discontinuity, was argued to be the driving force of ferromagnetism beyond the critical thickness. Here systematic first-principles calculations have been performed to check these mechanisms in ultrathin $LaMnO_3$ films as well as superlattices [2]. Starting from the very precise descriptions of both $LaMnO_3$ and $SrTiO_3$, it is found that the compressive strain is the dominant force for the appearance of ferromagnetism, while the open surface with oxygen vacancies leads to the suppression of ferromagnetism. Within $LaMnO_3$ layers, the charge reconstructions involve many competitive factors and certainly go beyond the intuitive polar catastrophe model established for $LaAlO_3/SrTiO_3$ heterostructures. Our paper not only explains the long-term puzzle regarding the magnetism of ultrathin $LaMnO_3$ films but also sheds light on how to overcome the notorious magnetic dead layer in ultrathin manganites.

[1] X. R. Wang, C. J. Li, W. M. L, T. R. Paudel, D. P. Leusink, M. Hoek, N. Poccia, A. Vailionis, T. Venkatesan, J. M. D. Coey, E. Y. Tsymbal, Ariando, and H. Hilgenkamp, Science 349, 716 (2015)
[2] M. An, Y.K. Weng, H.M. Zhang, J.-J. Zhang, Y. Zhang, and S. Dong, Phys. Rev. B 96, 235112 (2017)

First-principles modeling for $SrTiO_3$/Si interfaces

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The epitaxial deposition of oxides on silicon opens the possibility of incorporating their diverse properties into silicon-device technology. Growth of $SrTiO_3$ has received particular attention because of its large dielectric constant, thermodynamical stability in contact with Si, and potential ferroelectricity. Although deposition of $SrTiO_3$ on Si was first reported more than a decade ago, the exact atomic structure of the $SrTiO_3$/Si interface is still under debate. Moreover, definitive explanation of the influence of interfacial structure on electronic properties is still poorly understood. In this work, we systematically investigate $SrTiO_3$/Si interfaces from first-principles modeling in order to contribute to a better understanding of these issues.

The best-known method for growing epitaxial oxides on silicon requires the deposition of monolayer of an alkaline earth metal, usually Sr, as the initial step. However, the details, as well as the impact of defects on this process are not well understood. Using first-principles density functional theory calculations,we firstly analyze the electronic states of the (1×2) reconstructed Si(001) surface with half monolayer Sr coverage. Various types of defects, including arrays of Sr adatoms and rows of Sr vacancies, are taken into account. Their scanning tunneling microscopy (STM) images are presented and compared with recent experimental results.

Based on the thorough understanding of Sr/Si(001) surface, we further focus on the $SrTiO_3$/Si heterostructures. As we know, for the clean (001) surface of silicon, owing to a lack of upper bonding partners, pairs of silicon atoms dimerize, using up one dangling bond per atom to form the dimer bond. By depositing $SrTiO_3$, the structural complexity of both the ferroelectric $SrTiO_3$ itself and the buffer layers offers the possibility to break the 'dimer-row' reconstruction of silicon atoms. The driving force has been analyzed in details. Especially, in our first-principles calculations, the electrostatic coupling between the surface and the interface is taken into account.

This work helps to a fundamental understanding of the important role played by interfacial structures in the $SrTiO_3$/Si heterostructures, provides theoretical support for the interpretation of experimental reports, and may suggest guidelines for the future design of coupled functional oxide-semiconductor devices.

[1] Forst C. J. et al. Nature 427, 53-56 (2004).
[2] Reiner J. W. et al. Phys. Rev. Lett. 101, 105503 (2008).
[3] Tersoff J. & Hamann D. R. Phys. Rev. Lett. 50, 1998 (1983).
[4] Tersoff J. & Hamann D. R. Phys. Rev. B. 31, 805 (1985).
[5] Wang J. et al. Phys. Rev. B 60, 4968 (1999).
[6] Ashman C. R. et al. Phys. Rev. B 69, 075309 (2004).
[7] Vanpoucke D. E. P. & Brocks G. Phys. Rev. B 77, 241308 (2008).

Anomalous behavior in transverse resistivity in the itinerant ferromagnetic oxide $SrRuO_3$

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Phenomena giving rise to voltages transverse to electric currents, such as anomalous and topological Hall effects, have been at the heart of current condensed matter physics. Here, we show that epitaxial thin films of the itinerant ferromagnetic oxide $SrRuO_3$ exhibit anomalous transverse resistivity associated with magnetization reversal, which is reminiscent of the emergence of the topological Hall effect. The behavior of the anomalous transverse resistivity of $SrRuO_3$ films is found to depend on both the film thickness and the Ru vacancies. The anomalous peaking behavior in the transverse resistivity is enhanced when the film is atomically thin. Furthermore, films with fewer Ru vacancies exhibit no anomaly in transverse resistivity. Our observations imply that the Ru vacancies significantly influence on transverse resistivity in $SrRuO_3$. In this presentation, we also discuss the origin for the emergence of the anomalous peaking behavior in the transverse resistivity will be discussed.