



**UNIVERSITÉ  
DE GENÈVE**

**FACULTÉ DES SCIENCES**

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**LE DEPARTEMENT DE CHIMIE PHYSIQUE**

*a le plaisir de vous inviter à la*

**CONFERENCE**

*intitulée*

**FASCINATING PROPERTIES OF METAL-BORON-HYDROGEN  
SYSTEMS : FROM HYDROGEN STORAGE TO  
IONIC CONDUCTIVITY**

*donnée par*

**Prof. Zbigniew LODZIANA**  
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**le MARDI 4 OCTOBRE 2016 à 16h30**

**SALLE 1S081**  
**Sciences III**

**30 quai Ernest-Ansermet ou 4 bld d'Yvoy**

**Responsable : Prof. Hans HAGEMANN**

## **Fascinating properties of metal-boron-hydrogen systems: from hydrogen storage to ionic conductivity**

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Interest in materials related to energy storage brought up extensive studies of borohydrides ( $M(BH_4)_x$ ) – a potential hydrogen storage media due to high gravimetric content of  $H_2$ . Severe problems related to the reversibility of hydrogen absorption/desorption are still not fully solved, however these simple materials reveal interesting and unexpected properties. A high conductivity of cations in the solid state structures is the one that recently renew interest in metal borohydrides and their derivatives with large  $B_{12}H_{12}^{2-}$  or similar anions.

Examples of theoretical studies, based on DFT calculations, will be presented – covering problems related to structure, dynamics, thermodynamics and the ionic conductivity mechanism in compounds with  $BH_4^-$  and  $B_{12}H_{12}^{2-}$  anions.