SOCIÉTÉ CHIMIQUE DE GENÈVE

The art of solving approximately the Schrödinger equation for chemistry, biochemistry and materials science

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Immediately after introduction of the Schrödinger equation, almost one century ago, chemistry started benefitting from it. The concepts such as: chemical bonds, Lewis structure, delocalization, etc. got their mathematical interpretation. Such object as *molecular orbital* is omnipresent in reasoning of a chemist. With the emergence of computers, Schrödinger equation started being used also to make quantitative predictions. Solving it with accuracy, which surpasses that of experimental measurements, became reality for molecules comprising a few atoms. Unfortunately, modern chemistry deals with larger systems, for which solving Schrödinger equation with arbitrary accuracy is beyond reach of humanity. It is not due to limits in speed of computers but rather due to the intrinsic scaling properties of this equation.

Does it mean that one should abandon hope for using Schrödinger equation as the basic equation to simulate properties of chemical systems that comprise more than a few atoms? My personal answer is that not. There are approximate methods providing useful solutions for specific systems and problems (this is why “art” in the title). Actually, there are many such methods. They differ in their domain of applicability and the amount of additional (empirical) information needed before the simulation is made. So called multi-level methods emerge as one of most promising strategy. In 1993, we introduced the formalism (Frozen Density Embedding Theory) providing the common formal framework for various multi-level simulation methods. In this framework, we explore the fact that all information about the chemical system is contained in its *ground-state electron density*. Several groups adopted this formalism for their needs. I will overview our own recent simulations studies of the effect of microscopic environment on properties of embedded molecules: color of chromophores in proteins, UV/Vis spectra of chromophores in zeolites, and optical properties of impurities in solids, for instance. Time permitting, I will overview our other interests such as methods to extract chemical information (about aromaticity for instance) from electron density.

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La conférence est publique

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