Project 3.14 On the inclusion of magnetic interactions in hybrid QM/MM calculations for catalysis and spintronics

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Background:

Hybrid quantum chemical / molecular mechanics method (QM/MM) methods have become almost irreplaceable when computing properties of large chemical systems like proteins or supported catalysts. QM/MM allows for interdisciplinary breakthroughs when physics, chemistry, and computational computer science meet to produce new fundamental knowledge about the nanoworld. Within this approach, the core region is treated fully at the QM level with the possibility to apply high-level methods such as a state-of-the-art coupled cluster methods (see e.g. A. Kubas et al. J. Phys. Chem. Lett. 2016, 7, 4207). The rest of the system is treated approximately, typically as a set of point charges included in the QM Hamiltonian and, in many cases, responding to QM charge distribution. Although QM/MM method can yield excellent results in predicting local chemical reactivity, it has no apparatus to predict the long-scale quantum effects unless very large QM regions are accounted for. The latter, in most cases, renders the calculations too expensive. Our most recent development is the successful analytical model of the long-range electrostatic effects on metal surfaces. Here, the metallic surface states are divided into two parts: the typical deep bulk states, which aren't affected by the surface chemistry, and the second, a most significant part – the Tamm surface states. The analytical model allows for generating a point-charge field to be used in QM/MM calculations for catalytic reactions at metallic surfaces. However, the developed approach does not cover magnetic interactions within the system studies, which is a serious drawback when studying open-shell transition metals and their complexes at metallic surfaces important in catalysis and spintronics.

We expect the Ruderman-Kittel-Kasuya-Youside interaction to provide the driving force for the emergence of many phenomena in strongly correlated materials. The interaction of a localized magnetic moment with a metallic host gives rise to the Kondo many-body state. There is no real-space model of the interacting system of two magnetic moments placed on a Kondo or Kronig-Penney surface that would be easy to apply for quantum chemistry, yet this theoretical field is evolving fast, and one-dimensional Kondo chain study was published lately (Moro-Lagares et al., Nat. Com. 2019, 10, 2211). One has to rethink the current developments in the fields of spintronics, physics of conducting materials, and surface chemistry and build a simple model which will be an acceptable compromise of all theories combined with the necessary degree of theoretical accuracy.

The topic of the research will include the development of the purely theoretical mathematical approach with knowledge both from surface chemistry as well as physics of condensed matter and will be combined with state-of-the-art computational methods.

Aim:

To include Ruderman-Kittel-Kasuya-Youside interaction in the existing electrostatic analytical model that covers the response of a metallic charge density to the presence of adsorbed molecules.

Requirements:

- MSc in physics or related fields (mathematics, chemistry etc.),

- excellent knowledge of solid-state physics, physics of metals, functional analysis, and perturbation theory,
- knowledge of English that allows to communicate research and read the relevant literature,
- advanced knowledge of at least one programming or scripting language.