The 302nd MANA Seminar

Jointly with CMS

Simulation of charge transfer: from oxides to organic semiconductors to proteins

Chair: Dr. Yoshitaka Tateyama (Nano-System Computational Science Group)

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Charge transfer and transport plays a crucial role in many energy converting processes, both in the inorganic world as well as in biology. In this talk I will review some of the progress we have made in thecomputation of the parameters that determine the thermodynamics, kinetics and the mechanism of charge transport in condensed phase systems based on constrained and fragment orbital density functional theory methods. Applications we will discuss are hole transfer between oxygen vacancies in MgO, electron transfer in fullerene materials and in a deca-heme 'wire'-protein. We find that while for proteins, charge hopping models usually provide a good description, this is not the case for organic semiconductors. For the latter, the dynamics of the excess charge should not be integrated out, as is typically done in hopping models, but solved explicitely, e.g. via non-adiabatic dynamics methods. Oxide materials form an intermediate case, where charge hopping models are valid for tunneling distances that are larger than a certain critical defect separation but need to be replaced by an appropriate scattering (Green's function) approach for smaller distances. We expect that our findings will guide future modelling efforts of gate dielectrics in transistors, organic semiconductors for organic photovoltaics, and electron transporting proteins for use in biofuel cells.

Venue: **Auditorium, 1F, WPI - MANA Bldg.,**

Date: **December 14th, Friday** ***Time:*** **15:30-16:15**

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