IRTG-Joint Seminar

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“Interaction between molecules in a Cold Ensemble Matrix”

Photocurrent generation in organic photovoltaics (OPVs) relies on the dissociation of the excitons into free electrons and holes at donor/acceptor heterointerfaces. The low dielectric constant of organic semiconductors leads to strong Coulomb interactions between electron-hole pairs that should in principle oppose the generation of free charges. The exact mechanism by which electrons and holes overcome this Coulomb trapping is still unclear. Our goal is to gain a deeper understanding of the nature of CT excitons in a donor/acceptor interface as present in organic solar cells. Single donor/acceptor pairs may be trapped in cold hydrogen or rare-gas matrix, where spectra can be recorded in unprecedented precision. We aim to look precisely into the vibronic transitions important in CT excitons as their fingerprints. The theoretical approach in this study is Density Functional Theory (DFT) for the ground state and Time Dependent DFT (TDDFT) for excited states. The accurate description of van der Waals (vdW) interaction between molecules is needed also. In this presentation an overview on CT mechanism proposed since now is given and basic explanations on (TD)DFT methods and their applications in this field are discussed.

Tuesday, December 8th, 2015,

(UF) 6:00p.m., room 023, 1st floor, RZ, Hermann-Herder-Str. 10
(UBC) 9:00a.m., place: tba

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