HL 56: Invited Talk Xavier Blase

Time: Wednesday 9:30–10:00 Location: POT 006

Invited Talk HL 56.1 Wed 9:30 POT 006

Ab initio many-body perturbation theory for organic photovoltaics — •Xavier Blase — Institut Néel, CNRS and UJF, Grenoble, France

Initially developed in the mid-eighties at the ab initio level for inorganic semiconductors, a family of many-body perturbation theories, the so-called GW and Bethe-Salpeter (BSE) formalisms, have been shown recently to yield electronic and optical (excitonic) properties of bulk and gas phase organic systems with a remarkable accuracy. After introducing some of the important limitations associated with organic photovoltaic cells, we will show that key features, such as band gaps and offsets, bands dispersion, electron-phonon coupling strength, and donor-to-acceptor charge-transfer excitations, can be described with unprecedented accuracy by such techniques that are parameter-free and allow the study of systems comprising up to a few hundred atoms. Upcoming challenges, such as the development of specific embedding techniques that may account for dynamical long range screening in disordered dense organic phases, will conclude this presentation. The selected calculations have been performed with a recently developed Gaussian-basis GW and BSE package, the Fiesta code.

Selected references: I. Duchemin and X. Blase, Phys. Rev. B 87, 245412 (2013); I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. Lett. 109, 167801 (2012); S. Ciuchi et al., Phys. Rev. Lett. 108, 256401 (2012); C. Faber et al., Phys. Rev. B, 86, 155315 (2012); C. Faber et al., Phys. Rev. B 84, 155104 (2011).