nanoSeminar Series 2014

Institute for Materials Science

Prof. Dr. Xavier Blase

Institut Néel, CNRS and
Université Joseph Fourier, Grenoble, France

"Towards ab initio many-body perturbation theory for organic photovoltaics"

Thursday, May 15
13:00 – 14:00

Seminar Room 115, Hallwachsstr. 3 (HAL)

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 accurately described by such techniques that are parameter-free and allow the study of finite size or periodic systems comprising up to a few hundred atoms. Specific examples will be presented where the GW/BSE formalism outperforms existing density functional theory calculations with semilocal, global or range-separated hybrid functionals. Several challenges are however still ahead of such techniques, such as calculating excited states forces and phonons, or the development of specific discrete or continuous polarizable models. The selected calculations have been performed with a recently developed Gaussian-basis GW and BSE package, the Fiesta code.

Speaker's CV

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DRESDEN concept

complex nano materials

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Short CV:

After a Ph.D at UC Berkeley under the supervision of S.G. Louie, and a postdoctoral stay at EPFL with Roberto Car, X. Blase joined the French CNRS in 1996 in Lyon. He is now CNRS research director at Institut Néel in Grenoble. His domain of expertise is that of theory and ab initio simulations in condensed matter physics, applied to various systems and properties, from the structural and electronic properties of nanotubes and graphene to the superconducting transition in doped semiconductors. His main domain of study since 2011 concerns the development of efficient many-body perturbation theory tools for the study of the electronic and optical properties of organic systems