CFEL SCIENCE

SEMINAR

9th July 2014 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

Gabriel Bester

University of Hamburg, Physical Chemistry Department

Atomistic wavefunction-based methods for the calculation of the optical and dynamical properties of nanostructures

I will introduce our approach to nanoscopic systems, namely atomic effective pseudopotentials [1] (AEPs) coupled to the quantum chemical configuration interaction approach [2]. The combination of a quasiparticle based approach (AEPs) and a quantum chemical method is challenging, but allow us to treat realistic structures, i.e, many thousands of atoms, at a high level of accuracy [3] and without ad-hoc parameters.

While this solves, to a certain extent, the length-scale problem, we are now addressing the time-scale problem underlying the calculation of dynamical properties. I will show how we combine our atomistic ab-initio results to mesoscopic approaches and will illustrate it with the problem of the “phonon bottleneck”, i.e., how to bridge large electronic gaps with low energy vibrations [4].

* In collaboration with Peng Han, Ricardo Cardenas, Jun-Wei Luo, Alex Zunger, Ranber Singh and Jerome Jackson.

[1] R. Cardenas and G. Bester
Atomic effective pseudopotentials for semiconductors, Phys. Rev. B **86** 115332 (2012).

[2] G. Bester
Electronic excitations in nanostructures: An empirical pseudopotential based approach (Review), J. Phys. Cond. Mat. **21**, 023202 (2009).

[3] P. A. Labud et al.
Direct Quantitative Electrical Measurement of Many-Body Interactions in Exciton Complexes in InAs Quantum Dots, Phys. Rev. Lett. **112**, 046803 (2014).

[4] P. Han and G. Bester, submitted.

Host: Robin Santra - CFEL Theory Division