CFEL SCIENCE

SEMINAR

21st June 2017 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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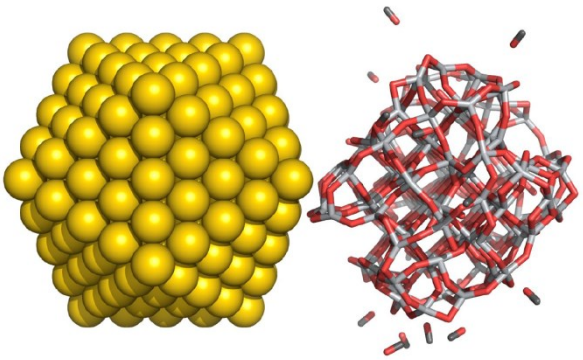
DFTB+ - An approximate DFT method: Applications to excited state simulations of nanomaterials

The new release of DFTB+ as a density-functional (DFT)-based approach, combining DFT-accuracy and Tight-Binding (TB) efficiency, is reported; http//:www.dftb.org. Methodological details and recent extensions to improve reliability and accuracy will be described. Advanced functions include spin degrees of freedom, time dependent methods for excited states, non-adiabatic electron-ion dynamics and quantum transport calculations under open boundary conditions using non-equilibrium Green´s function methods.

The major focus of the talk will be on the TD-DFTB extensions and implementation in linear response and in the real time domain. In the linear response excited state absorption spectra of nitric oxide TiO2-nanoparticle hybrids will be calculated revealing formation of charge transfer complexes on TiO2 as new source for visible light activity. In addition the TD-DFTB implementation in time domain allow to study the interaction of ultra-short laser pulses with nanomaterials and hybrid interfaces and to follow the coupled electron-ion dynamics in non-adiabatic molecular dynamics simulations. Applications to laser-induced ultra-fast hot electron injection from metal nanoparticles into adsorbed molecules for driving catalytic reactions will be demonstrated. As example the Au-TiO2-CO hybrid structure is shown below.



Host: Robin Santra – CFEL-DESY Theory Division