ANNOUNCEMENT

UNIVERSITÄT SALZBURG

Vortragsankündigung

Mittwoch, 22. Mai 2019, 11.15 Uhr

Seminarraum I (JAK2AOG1.33), Jakob-Haringer-Straße 2a

Prof. Dr. Thomas FRAUENHEIM
Bremen **C**enter for **C**omputational **M**aterials **S**cience
http://www.bccms.uni-bremen.de

"Atomistic modeling of quantum processes in nanoscale devices"

The new release of DFTB+ as a density-functional (DFT)-based approach, combining DFTaccuracy 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, nonadiabatic 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 time-dependent DFTB extensions. I am going to present the first real-time atomistic simulation of the quantum dynamics of plasmon excitations in icosahedral silver nanoparticles under strong laser.

The TD-DFTB implementation in real time domain also allow to simulate transient absorption spectra (TAS) fully atomistically. When this technique is applied to the study of ultrafast dynamics of Soret-excited zinc(II)-tetraphenylporphyrin in the sub-picosecond time scale, quantum beats in the transient absorption caused by impulsively excited molecular vibrations are observed. As last example ultrafast electron transfer in P3HT-PBCM organic blends will be demonstrated to become enhanced by the nuclear motion and under open boundary conditions with applied bias, see example below.