



TECHNISCHE UNIVERSITÄT  
CHEMNITZ

# Institut für Physik Physikalisches Kolloquium



Mittwoch, 11.04.2018, um 16:00 Uhr

Ort: Reichenhainer Str. 90;  
Zentrales Hörsaal- und Seminargebäude,  
Raum 2/N013

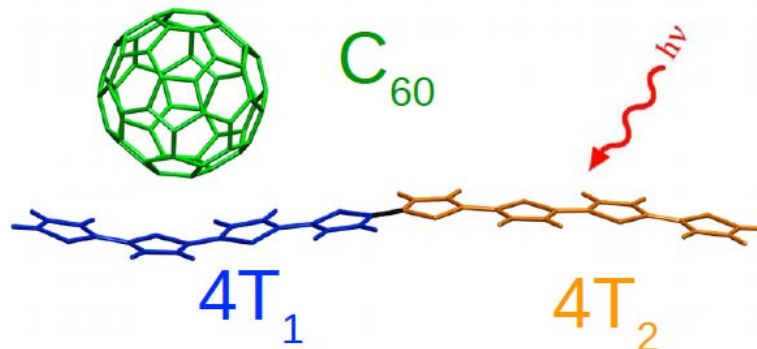
**Prof. Dr. Thomas Frauenheim**  
Universität Bremen

## Atomistic modeling of quantum processes in nanoscale devices

DFTB+: Applications to device and 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 time-dependent DFTB extensions and implementation of the electron-photon interaction for studying photo-voltaic and optoelectronic devices. In addition the TD-DFTB implementation in real 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 and ultrafast electron transfer in P3HT-PBCM organic blends will be demonstrated. **As example the 4T - C60 hybrid structure is shown below.**



Alle Zuhörer sind ab 15:45 zu Kaffee und Tee vor dem Hörsaal eingeladen.

Informationen zum Vortrag erteilt:

Prof. Dr. Dr. h.c. D.R.T. Zahn, Tel. 0371 531 33036



[www.tu-chemnitz.de/physik](http://www.tu-chemnitz.de/physik)