TECHNISCHE UNIVERSITÄT DRESDEN

Bereich Mathematik und Naturwissenschaften Fakultät Physik

PHYSIKALISCHES KOLLOQUIUM

Referent: **Prof. Dr. Thomas Frauenheim**
Bremen Center for Computational Materials Science,
University of Bremen

Thema: **Atomistic modeling of quantum processes in nanoscale devices**

Zeit und Ort: Dienstag, 11.12.2018, 16:40 Uhr
Recknagel-Bau, Hörsaal REC/C213, Haeckelstr. 3

Leiter: Prof. Dr. Matthias Vojta

Kurzfassung: 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 developments of this approach started at TU-Dresden in the mid-eighties by Helmut Eschrig and Gotthard Seifert. Nowadays 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. I am going to present the first real-time atomistic simulation on the quantum dynamics of plasmon excitations in icosahedral metal nanoparticles under strong laser pulse irradiation. We identify the emergence of sub-picosecond breathing-like radial oscillations starting immediately after laser pulse excitation, with increasing amplitude as the field intensity increases. The ultrafast dynamic response of nanoparticles to laser excitation points to a new plasmon assisted mechanism rather than longer time-scale equilibrium electron-phonon scattering previously assumed.

Biographie: Thomas Frauenheim has made his PhD in 1976 and his Habilitation in 1982 at Technical University Dresden. As Postdoc he has worked 5 years in the Joint Institute for Nuclear Research in Dubna until 1982. Later, in 1998 he accepted an offer as chair professor in Computational Materials Science from University of Paderborn and in 2006 he moved to University of Bremen to become the founder of the Bremen Center for Computational Materials Science. Since the mid-90th he pioneered the development of the density-functional based tight-binding method (DFTB) which combines the high efficiency of semi-empirical methods with the accuracy of ab initio density-functional theory (DFT). As director of the German CECAM-Node Multi-scale modelling from 1-st principles since 2009 he has initiated noumerous International CECAM-Workshops and hands-on-tutorials on atomistic simulations bringing together world leading experts and young researchers from computational solid state and materials physics, theoretical chemistry and molecular biology.

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