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Self-energies: Opening Doors for Nanotechnology

State of the art nanodevices have reached length scales in which a clear distinction of fundamental physics, material science and device engineering is not applicable. Reliable performance predictions of nanodevices have to embrace all these fields: coherent quantum mechanical effects such as tunneling, confinement and interferences, atomistic effects such as strain profiles, alloy compositions and interface relaxations, uncertainty effects such as incoherent scattering on phonons and device imperfections and electrostatic effects have all similarly strong impact on the nanodevice performances. Many of these aspects are described in different physical models and are characterized on different length scales.

In this talk, it will be shown how the concept of self-energies can be used to interface all these fields into the same nanotechnology modeling framework. Self-energies are most commonly used in the quantum transport method of nonequilibrium Green's functions (NEGF). The NEGF method is widely accepted as the most consistent method for modeling coherent and incoherent effects. Given that this method allows for atomic resolution and the inclusion of strain effects, alloy disorder and electrostatics, it is most often used for charge, heat and spin transport in nanometer scaled systems. Nevertheless, it will be shown how self-energies can get used beyond NEGF. It is also part of this talk how self-energies can set nanotechnology into the context to solve 3 of mankind's biggest challenges: shortage of energy, shortage of fresh water and the decline of world's economy.

About the presenter

Tillmann Kubis graduated to PhD at the Technische Universität München (Germany) in theoretical semiconductor physics in 2009. He is currently working as Research Assistant Professor in the network for computational nanotechnology of Purdue University. His work includes development and implementation of new algorithms in the framework of general quantum transport within the nonequilibrium Green's function method. His algorithms are published in the academic open source semiconductor nanodevice modeling tool NEMO5. This code is used among many academic and industrial groups including Intel, Samsung, Lumileds, and TSMC. His research currently applies to electron and phonon transport, tight binding parameter extraction from density functional methods, spin transport with topological insulators and design optimizations of terahertz quantum cascade lasers and nitride based light emitting diodes.

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**Monday, April 4,
2016**

**09:30 AM Seminar
Room WANG 1004**