

Physics Colloquium

Michigan Technological University

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Room 13, Fisher Hall

Ab-initio Assisted Process and Device Simulation for Nanoelectronic Devices

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Abstract

The continuing miniaturization of traditional semiconductor devices deep into the nano-realm and novel concepts such as molecular devices require an unprecedented attention to the detailed geometry and electronic properties on the atomic scale. This talk will examine the role of atomistic modeling – mostly on the basis of quantum mechanical *ab-initio* methods – for current and future semiconductor process and device simulations.

First, we will discuss atomistic enhancements of traditional process modeling to include nano-scale effects and the nanoscale characterization problem for conventional devices, where traditional characterization techniques cannot provide the needed information anymore. We discuss a coupled experimental-theoretical approach based on analytical transmission electron microscopy techniques (Z-contrast spectroscopy and electron energy-loss spectroscopy) that can detect single dopant atoms and even allow to “see” the atomic structure of amorphous oxide layers. With this method, we could identify for the first time an “ideal” interface between Si:Ge and SiO₂.

Finally, we will discuss simultaneous process and electron-transport modeling on the atomic scale for the example of a carbon nanotube Schottky device with titanium leads. Whereas several groups have suggested ways to study electron transport through molecular devices, few concepts exist to date how to determine sensible finite-temperature contact structures between molecule and the contacting metal. We propose using *ab-initio* accelerated dynamics methods to study contact evolution and examine the considerable influence of the contact structure on the electron transport.

Biography

Wolfgang Windl is an Associate Professor in the Department of Materials Science and Engineering at The Ohio State University since October 2001 and works in the area of Nanoscale Computational Materials Science. His field of expertise is in the area of atomistic simulations, especially within density-functional theory. Currently, he mostly works on nanostructured interfaces and molecule-surface interactions of semiconductor device systems. Previously, he spent four years with Motorola, first as Senior Staff Scientist in Motorola’s Computational Materials Group at Los Alamos National Laboratory, and later as a Principal Staff Scientist in the Digital DNA Laboratories in Austin, TX, where he was working in the area of multiscale modeling of semiconductor processing. Before that, he held postdoctoral positions at Los Alamos National Laboratory and Arizona State University. He received his diploma and doctoral degree in physics from the University of Regensburg, Germany. He is co-recipient of 1998 and 1999 Patent and Licensing Awards from Los Alamos National Laboratory for his contributions to the molecular modeling code CLSMAN (with Arthur Voter, Robert Walker, and Joel Kress) and of the 2004 Nanotechnology Industrial Impact Award from the Nano Science and Technology Institute for the discovery of atomically sharp “perfect” interfaces in semiconductor gate stacks (with Gerd Duscher).

