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Quantum Transport Simulation for 21st Century Electronics

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Wednesday, February 23, 2022
10:30 AM • WANG 1004

Zoom info: https://purdue-edu.zoom.us/j/92952701304 ~Meeting ID: 929 5270 1304

Abstract

Device simulation plays a major role in the electronics industry reducing development time and cost by replacing costly repetitions of fabrication and benchmarking experiments. The continued miniaturization in the Moore's law era has led us to devices with atomic scale dimensions requiring quantum mechanical simulation tools for reliable predictive modeling.

This talk has two parts. First, I will outline the methods we have developed at Purdue which have set new nanodevice simulation standards in industry: The first derivative of our quantum code library, NEMO5, had been adapted by the semiconductor companies intel, TSMC, Samsung, and others. as the nanotransistor simulation standard. My quantum transport methods are deeply embedded in several industrial simulation engines most notably at Intel and Silvaco. Academic researchers too have adapted the code for their device and material predictions. Every year, more than 25,000 simulations are performed with it on nanohub.org alone.

In the second part of this talk, I will describe how we are currently expanding the quantum transport methods and the quantum code library in collaboration with chemists at Purdue and Merck towards molecular chemistry, material crystallization, drug formulation and amorphous material research. Our vision is to expand the impact of our quantum transport models from the electronics industry to the chemical and pharmaceutical industries.

Bio

Tillmann Kubis is currently the Silvaco Research Assistant Professor in the Elmore Family School of Electrical and Computer Engineering. He received his PhD from the Technische Universität München (Germany) in theoretical semiconductor physics in 2009. His early quantum transport software powers the quantum cascade laser, resonant tunneling diode and quantum well functionality of the commercial software nextnano. Since 2011, he has been working on developing quantum transport methods and their numerically efficient implementation in highly scalable, industrially relevant simulation tools collaborating with many semiconductor companies (Intel, Samsung, TSMC, Lumileds, IBM, GlobalFoundries, Hamamatsu Optics, Silvaco) on predicting charge, heat, and spin transport in semiconductor nanodevices, optoelectronics, 2D materials and topological insulators. Tillmann Kubis is core developer of Purdue's quantum code library and since 2018 has been leading NEMO5 development and its commercialization through Silvaco. Tillmann Kubis is codeveloper of the ideas to innovation class sequence of the professional master's program in the Elmore Family School of Electrical and Computer Engineering.

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