MS6
Fast Reaction-Diffusion of Defects in Cadmium Telluride

In this talk, we discuss the asymptotic behavior of a reaction-diffusion system with extremely fast reactions. We use a perturbation method to derive a limiting equation for a simple reaction network and present numerical results for a more complicated model with a scheme derived from a bimolecular kinetic reaction model. Finally, we briefly discuss asymptotic preserving schemes for Cadmium Telluride Solar Cells. Cadmium Telluride is the leading silicon alternative for consumer solar cells. The behavior of the device can be modeled as a reaction-diffusion equation for charged carriers with a self-consistent coupled electric field. In the course of device production additional elements (such as Chlorine and Copper) are added to the device. These molecules enter the device as diffusing interstitial defects, but can react nearly instantaneously with the CdTe lattice. To better understand the fabrication of such devices, we must first understand this physical process.

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MS6
Electron Transport in Nanostructures: Physical Models and Numerical Methods

Research on electron devices scaling at the 5 nm gate-length has triggered a growing interest on two-dimensional (2D) materials, even beyond carbon-based electronics. Among them, transition metal dichalcogenides (TMDs), silicene, germanene, phosphorene, stanene, and topological insulators. Here we will focus on the use of pseudopotentials to treat the electronic structure of systems at the nanometer scale (2D crystals, nanowires, nanoribbons), their stability and properties, and to study electronic transport, both semiclassically (mobility, Monte Carlo) and from a quantum perspective (open systems). The former task requires fast matrix-free eigenvalue solvers and I will briefly show how our use of the Residual Minimization Method-Direct Iteration in Iterative Subspace (RMM-DIIS) and fast-Fourier transforms has been used to calculate the tunneling current between large graphene nanoribbons. Pseudopotential-based quantum transport, on the other hand, requires not only the implementation of sophisticated physical transport models, but also the solution of very large linear systems. We will present our formulation of the problem and results of the simulation of field-effect transistors with graphene nanoribbons and Si nanowires as active channels. Finally, we will discuss the mathematical formulation of a related problem, namely, the calculation of the dielectric response (or, simply put, of the position-dependent dielectric constant) of the nanostructures of interest.

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MS6
Modeling Spin-Dependent Phenomena for New Device Applications

To enhance performance and to reduce energy consumption, electron spin is investigated as replacement of electron charge for storage and computation in future electronic devices. In contrast to charge, spin is not conserved but relaxing to its equilibrium zero value. In the case of semiconductor films, technologies are needed to boost the spin lifetime to make the technology feasible. In silicon films the spin lifetime is determined by intervalley scattering. Applying stress appropriately decreases this undesired scattering effect, which should reduce the spin relaxation [Sverdlow and Selberherr, Phys. Rep. 585, 2015]. To confirm, we solve numerically the quantum mechanical description of the behavior of spin by calculating the wave functions and the scattering matrix elements via solving a kp Hamiltonian with spin-orbit interaction. For the computation of spin relaxation, the momentum dependence of the wave functions due to spin-orbit coupling responsible for spin admixture must be preserved, which significantly increases the demands for computational resources and requires extensive code parallelization. We predict a significant spin lifetime increase with appropriate viable stress. A universal behavior of the spin lifetime on the spin injection orientation is also obtained, with even a two times increase for a more complicated model with a scheme derived from asymptotic preserving schemes for Cadmium Telluride [Sverdlow and Selberherr, Phys. Rep. 585, 2015]. To confirm, we solve numerically the quantum mechanical description of the behavior of spin by calculating the wave functions and the scattering matrix elements via solving a kp Hamiltonian with spin-orbit interaction. For the computation of spin relaxation, the momentum dependence of the wave functions due to spin-orbit coupling responsible for spin admixture must be preserved, which significantly increases the demands for computational resources and requires extensive code parallelization. We predict a significant spin lifetime increase with appropriate viable stress. A universal behavior of the spin lifetime on the spin injection orientation is also obtained, with even a two times increase.
In this talk I will review some network centrality and communicability measures based on walks. These measures can be given an elegant closed form in terms of functions of the adjacency matrix. I will introduce the notion of total communicability of a network as a measure of network connectivity and robustness and show that it can be computed very quickly even for large graphs. Finally, I will discuss efficient edge modification strategies (including edge removal, addition, and rewiring) that can be used to obtain networks with desirable communicability properties. The talk is based on recent work in collaboration with Christine Klymko (LLNL) and Francesca Arrigo (Strathclyde).

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MS7
Influence Prediction for Continuous-Time Information Propagation on Networks Using Graph-Based Fokker-Planck Equation

We consider the problem of predicting influence, defined as...