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Design of Nanostructured Materials for Electronic, Thermoelectric, and Optoelectronic Applications[1]

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There is a large interest in tailoring semiconductor nanostructures to display desired electronic, thermal, or optical properties. Nanostructure dimensions are typically between a few and a few hundred nanometers, so they are too large to treat using atomistic methods, yet too small for continuum techniques. Their characteristics are strongly influenced by the properties of the interfaces, such as roughness, surface defects, or adsorbed charges. A major challenge in predicting the properties of nanostructures lies precisely in capturing the complex interplay between the confined particle states and the surface condition. I will review techniques typically used to analyze and predict the electronic, thermal, and optoelectronic properties of semiconductor nanostructures, with particular focus on the verstatility that the ensemble Monte Carlo technique offers in simulating these different transport phenomena. In particular, I will present our results on electronic and thermal transport in nanowires, based on the coupled electronic and thermal ensemble Monte Carlo simulation with confined electron and phonon dispersions. We will take a close look into boundary scattering of electrons and phonons, and features such as phonon localization, and discuss where atomistic simulations naturally come to play to aid in the desription of interfaces. We will then look into the design on strain superlattices for thermoelectric applications and the design of nanowire interfaces for tailoring thermal conduction. We will also examine how efficient transport simulation aids in the design of quantum cascade lasers. Multivalley ensemble Monte Carlo simulation, combined with k.p bandstructrue calculations and the dielectric continuum model, captures the transport of heat and charge in midinfrared quantum cascade lasers, and helps pinpoint the flaws of a laser design and directions for performance improvement through minimized leakage. We also discuss some promising new avenues, such as the simulaiton of high-frequency and transient phenomena in nanostructures using a combination of full electrodynamics together with the transport of charge and heat, from low- temperature ballistic to room-temperature diffusive transport regimes.

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