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**Multi-scale modeling of nanotransistors** ANDERS BLOM, KURT STOKBRO, QuantumWise A/S — This talk will discuss the current state-of-the-art in atomic-scale modeling of electronic devices. Over the last decade, combined DFT and NEGF methods have become an established approach for describing the non-equilibrium transport properties of e.g. nanotubes, graphene, and molecular electronics structures, involving system geometries with two leads, or electrodes. The ballistic tunneling current through the scattering or contact region can be computed at a finite bias applied between these electrodes. In order to simulate more device-like geometries it is however also necessary to consider the influence of various types of electrostatic gates and dielectric screening regions. To describe such systems realistically also requires a dramatically larger simulation cell, since the gates are typically positioned at distances that are an order of magnitude larger than the features of the active nanoscale device region itself. We will present how a multi-scale approach which includes an advanced description of the electrostatic environment, as implemented in the atomic-scale modeling platform Atomistix ToolKit from QuantumWise, can be used to model nanoscale field-effect type transistor structures and single-electron transistor devices.

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