Towards Realistic Atomic-Scale Modeling of Nanoscale Devices

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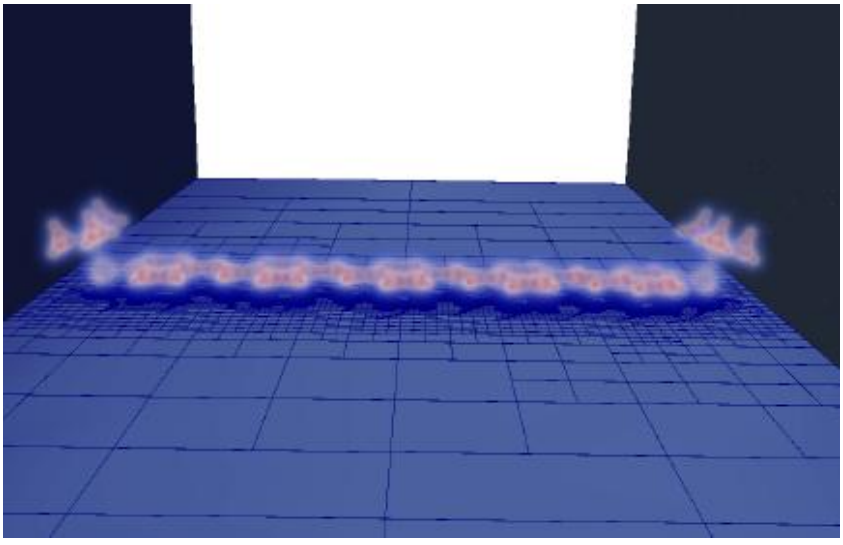
Although electronic device dimensions are rapidly approaching the nanoscale, their dimensions are still large from an atomistic perspective. Certain systems can still be studied with current state-of-the-art technology since the problems are relatively localized, such as interfaces and the effects vacancies or defects in them can have on Schottky barriers and interface resistance. For other properties, such as the influence on the transport and transistor characteristics of the electrostatic environment induced by gate electrodes, the simulation volume and atom count grows rapidly, however.

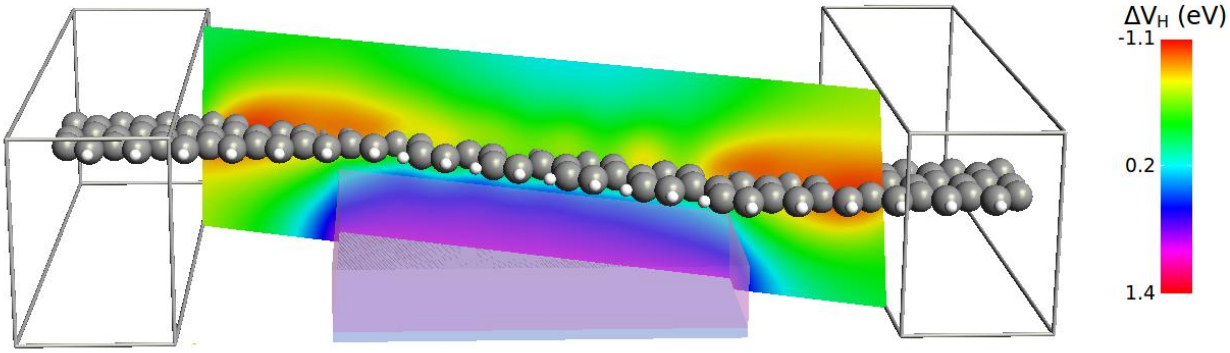
Therefore, a novel methodology is required in order to scale down current modeling techniques used within TCAD to be able to take into account atomic-scale effects. In this presentation we will present the current state-of-the-art in first-principles device modeling, as implemented in our software Atomistix ToolKit (ATK), and give an outlook to the challenges that lie ahead when scaling up the atomic-scale methods to more realistic dimensions.

We will discuss our recent progress in this area, including efficient Green's function evaluation and parallelization strategies based on block diagonalization techniques and the Krylov subspace method [1,2], the use of scattering states for improved performance of finite bias transport calculations [3], finite-element techniques coupled to first-principles calculations [4], and multi-scale models that take advantage of methods that operate on different complexity levels and length scales [4-6].

[1] D. E. Petersen, H. H. B. Sørensen, P. C. Hansen, S. Skelboe, and K. Stokbro, Journal of Computational Physics **227**, 3174-3190 (2008)
[2] S. Skelboe, The Scheduling of a Parallel Tiled Matrix Inversion Algorithm, submitted (2010)
[3] H. H. B. Sørensen, P.C. Hansen, D.E. Petersen, S. Skelboe, and K. Stokbro, Phys. Rev. B **79**, 205322 (2009)
[4] J. Avery, Ph.D. Thesis (2011)
[5] K. Stokbro, Journal of Physical Chemistry C, part of the "Mark A. Ratner Festschrift" (2010)
[6] K. Stokbro, D. E. Petersen, S. Smidstrup, M. Ipsen, A. Blom and K. Kaasbjerg, Phys. Rev. B **82**, 075420 (2010)



OPV5-tBu molecule in a single electron transistor environment, colored by the effective potential. This close-up view of the molecule illustrates the extremely high level of detail in the region where the electron density is large. [4]



Graphene nanotransistor consisting of two metallic zigzag nanoribbons connected by a semiconducting armchair ribbon. The nanoribbons are passivated with hydrogen, and the width of the ribbons are is 7 Å. The device is sitting on top of a dielectric and the transport is controlled by an electrostatic backgate. [6]