

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

High-resolution $O(N)$ DFT method and its application to large-scale nanowire simulations¹ JEAN-LUC FATTEBERT, SEBASTIEN HAMEL, Lawrence Livermore National Laboratory, GIULIA GALLI, UC Davis — Using a real-space finite difference discretization and orbitals localization techniques, accurate $O(N)$ Density Functional Theory calculations of systems made of thousands of atoms are now possible [1]. Using that methodology, we have investigated the static dielectric properties of silicon nanorods for diameters as large as 5 nm. We used a finite electric field method with non-periodic boundary conditions to calculate the dielectric response of the system, extending a previous study [2] to larger nanowires.

[1] J.-L. Fattebert and F. Gygi, Phys. Rev. B 73, 115124 (2006)

[2] S. Hamel et al., Appl. Phys. Lett. 92, 043115 (2008)

¹This research is supported by the Office of Science, U.S. Department of Energy, SciDAC Grant DE-FC02-06ER46262. Prepared by LLNL under Contract DE-AC52-07NA27344.

Jean-Luc Fattebert
Lawrence Livermore National Laboratory

Date submitted: 27 Nov 2009

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