High-resolution O(N) DFT method and its application to large-scale nanowire simulations\textsuperscript{1} 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 \cite{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 \cite{2} to larger nanowires.

\textsuperscript{1}This 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.

\textsuperscript{1} J.-L. Fattebert and F. Gygi, Phys. Rev. B 73, 115124 (2006)
\textsuperscript{2} S. Hamel et al., Appl. Phys. Lett. 92, 043115 (2008)