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Effects of Nonlocal Exact Exchange on Electrons in Core/Shell Nanowires BRYAN WONG, Materials Chemistry Department, Sandia National Laboratories, Livermore, California, ANDREW LONG, Department of Materials Science and Engineering, University of Illinois at Urbana Champaign, Urbana, Illinois — The unique properties of semiconducting heterostructure nanowires hold great promise for their incorporation in next-generation transistors, circuits, and nanoscale devices. The reduction in dimensionality produced by confining electrons in these heterostructure nanowires results in a dramatic change in their electronic structure, leading to novel properties such as ballistic transport and conductance quantization. In order to understand the formation of electron gases in core-shell nanowires, we developed a new pseudospectral approach for incorporating many-body, nonlocal exact exchange interactions within a self-consistent Schrodinger-Poisson formalism. Our approach is efficiently implemented in the open-source software package PAMELA (Pseudospectral Analysis Method with Exchange & Local Approximations) that can calculate electronic energies, densities, wavefunctions, and band-bending diagrams. Furthermore, in order to present a general-purpose set of tools that both experimentalists and theorists can easily use to predict electron gas formation in core-shell nanowires, we document and provide our efficient and user-friendly PAMELA source code that is freely available at http://alum.mit.edu/www/usagi.

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