

Abstract for an Invited Paper
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Nanocrystals, Nanowires and the Role of Quantum Confinement¹

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One of the most challenging issues in materials physics is to predict the properties of matter at the nanoscale. In this size regime, new structural and electronic properties exist that resemble neither the atomic, nor solid state. By changing the size of the system, inherently intensive properties become extensive properties, which can be strongly altered from the macroscopic limit. Such properties can have profound technological implications, e.g., at small length scales a poor optical material like silicon can be converted to an optically active one. Unfortunately, the development of theoretical methods to predict the properties of these systems is formidable challenge. Nanoscale systems may contain thousands of electrons and atoms, and often possess little symmetry. I will illustrate some recent advances in this area based on methods that are designed to exploit high performance computational platforms. I will present real space pseudopotential techniques for solving the electronic structure problem within density functional theory (see <http://www.ices.utexas.edu/parsec>). I will apply these techniques to systems ranging from clusters of a few dozen atoms to systems containing over a thousand atoms. I will present predictions for the structural and electronic properties of semiconductor nanowires and nanocrystals, intrinsic and doped, and will resolve some outstanding issues in the literature.

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