Predicting the electronic properties of 3D, million-atom semiconductor nanostructure architectures

A. Zunger, A. Franceschetti, G. Bester,
Materials Science Center, NREL.
W.B. Jones, Kwiseon Kim and P. A. Graf,
Scientific Computing Center, NREL.
L-W. Wang, A. Canning, O. Marques, C. Voemel
Computational Research Division, LBNL.
J. Dongarra, J. Langou and S. Tomov
Dept. of Computer Science, University of Tennessee.

corresponding author's e-mail address: acanning@lbl.gov

Abstract: The past ~10 years have witnessed revolutionary breakthroughs both in synthesis of

calculated using a superposition of screened atomic potentials which are fitted to the experimental band structure and LDA wavefunctions. Once we have calculated the potential we need to define a basis set in which the single particle Schrödinger equation will be solved. We have developed two different methods, one that uses a simple planewave basis set up to a certain energy cut-off (ESCAN[2]) and the other which uses a linear combination of strained bulk bands (SLCBB[3]). The single-particle Schrödinger equation is then solved as an interior eigenvalue problem, i.e. only a few eigenstates near the band gap are computed using the folded spectrum method. Once the single-particle energies and wave functions have been obtained the next step is to calculate the electronic excitations of the quantum dot. This task is accomplished using the configuration interaction (CI) method after first calculating the Coulomb and exchange integrals. Finally we calculate different

Figure 3: Correlation function for two electrons in a CdTe/CdSe nano dumbbell (~6,000 atoms). One electron is fixed at the center of the CdSe wire (white circle). The second electron is localized in the CdSe wire if electron-electron correlations are neglected and in the CdTe dots if correlation effects are included. This illustrates the importance of many-particle effects in describing the electronic properties of complex nanostructure architectures.

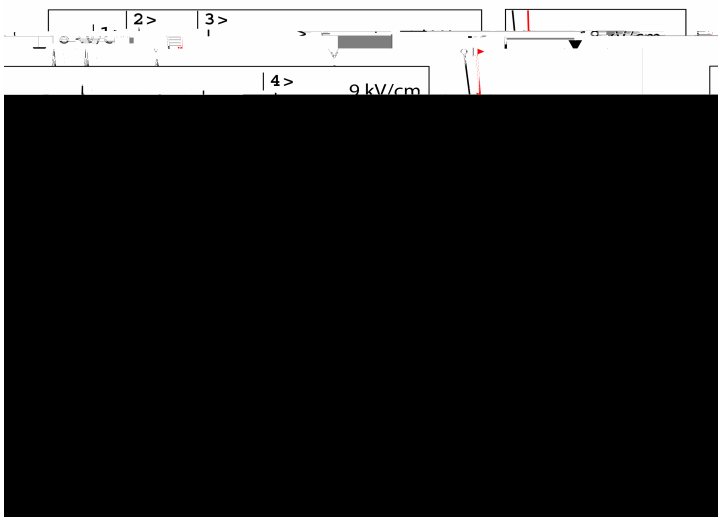

Figure 4: Calculated photoluminescence spectrum from a quantum dot molecule made of two vertically stacked InGaAs quantum dots as a function of the electric field. Degree of entanglement of the bright excitons as a function of electric field (left figure). At the field of -5.4 kV/cm the entanglement is maximized and reaches 80%. At this field, the state |1> anticrosses with states |2> and loses its oscillator strength. This gives a clear optical signature of entanglement. The dots contain about 50,000 atoms each and the complete system including the host barrier material contains about 1.6 million atoms.

finding 10 eigenstates corresponding to the highest VBM states for four CdSe quantum dots of increasing size from 39 to 1061 atoms. More details of this work can be found in references [10,11].

Figure 6: