Atomistic Modeling of Excitonic States in Semiconducting Nanostructures: Beyond 10-Million Atoms in Simulation

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Numerical calculations of excitonic properties of novel nanostructures such as nanowires [1], nanowire quantum dots [2], or crystal phase quantum dots [3] must combine atomistic accuracy with an approachable computational complexity. The key difficulty comes from the fact that excitonic spectra details arise from atomic scale contributions that must be integrated over a large spatial domain containing a million of atoms and more. In this work we present a step-by-step solution to this problem: combined empirical tight-binding, Hartree-Fock and configuration interaction scheme that unites linearly scaling computational time with the essentials of the atomistic modeling. First, we illustrate our method on the exampx of wellstudied self-assembled InAs/GaAs quantum dot, with the emphasis on the dark exciton spectra [4,5]. Next, we study excitonic properties of several nanostructures such as nanowire quantum dot molecules, quantum dashes, and natural quantum dots [6]. Finally, we show results of our approach applied to crystal phase quantum dots [7] containing more than 10 million atoms.

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