Atomistic Modeling of Multimillion Atom Nanostructures

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We present atomistic methodology for calculation of electronic and optical properties of multimillion atom nanostructures. This methodology combines the valence force field method for calculation of strain, the tight-binding method used to obtain single particle spectra and finally the configuration interaction method applied to calculate multi- and charged exciton energy and optical spectra. We illustrate our method on several examples including multiexciton complexes in self-assembled InAs/GaAs and charged excitons in InAs/InP quantum dots. We demonstrate necessity of atomistic calculation in such systems. We also discuss theoretical and numerical difficulties we had to overcome during the process of creation of the numerical programs package and issues related to high power computing involved in the calculation process.