ATOMISTIC MODELING OF MULTIMILLION ATOM NANOSTRUCTURES

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Atomistic calculations of properties of self-assembled quantum dots (SAD) involve computational domains of millions of atoms and their electronic properties cannot at present be computed using ab-initio methods. We present here [1] approach consisting of three major steps: (1) calculation of equilibrium positions of atoms using valence force field model (VFF), (2) calculation of single particle electron and hole states using the linear combination of atomic orbitals - tight binding approximation (TB), and (3) inclusion of interactions between quasi-particles by defining an effective Hamiltonian of interacting excited quasi-particles, solved using the configuration interaction method (CI).

In the VFF calculation we use the Keating model with material parameters chosen to reproduce bulk elastic constants. The TB parameters for InAs, InP and GaAs are obtained by fitting TB bulk band edges and effective masses to those obtained in experiment or by ab-initio calculations, with the valence band offset built into the parameter set. The strain dependence of TB parameters is fitted to reproduce the dependence of band edges on lattice deformation computed using DFT [2]. The Coulomb matrix elements for CI are obtained with TB wave functions involving \( \sim 10^8 \) orbitals, with on-site and nearest-neighbour terms computed by approximating the TB basis with Slater orbitals. In the CI step, typically \( \sim 10^4 \) configurations are used as a basis for each multi-exciton system, while emission spectra are calculated from Fermi’s Golden Rule.

We illustrate the method by computing the electronic and optical properties of a lens-shaped and disc-shaped InAs/InP/GaAs SAD using the VFF approach for 100s of millions of atoms, the 20-band sp3d5s* tight-binding model for millions of atoms and energies, states and emission spectra from up to ten multiexciton complexes obtained in the configuration-interaction method.