Study of Alloy Disorder in Quantum Dots through Multi-million Atom Simulations

Gerhard Klimeck*, Fabiano Oyafuso*, Timothy B. Boykin**, R. Chris Bowen*, P. von Allmen*, and Seungwon Lee*
* Jet Propulsion Laboratory
4800 Oak Grove Dr. MS 169-315, Pasadena, CA, 91109, gekco@jpl.nasa.gov
** University of Alabama at Huntsville, Huntsville, AL, USA

A tight binding model which includes s, p, d, and s* orbitals is used to examine the electronic structures of an ensemble of dome-shaped InGaAs quantum dots. Given ensembles of identically sized quantum dots, variations in composition and configuration yield a linewidth broadening of less than 0.35 meV, much smaller than the total broadening determined from photoluminescence experiments. It is also found that the computed disorder-induced broadening is very sensitive to the applied boundary conditions, so that care must be taken to ensure proper convergence of the numerical results. Examination of local eigenenergies as functions of position shows similar convergence problems and indicates that an inaccurate resolution of the equilibrium atomic positions due to truncation of the simulation domain may be the source of the slow ground state convergence.