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Atomistic Simulations of Long-Range Strain and Close-Range Electronic Structure in Self-Assembled Quantum Dot Systems. GERHARD KLIMECK, Network for Computational Nanotechnology, Purdue University, W. Lafayette, IN 47907, SHAIKH AHMED, MAREK KORKUSINISKI, SEUNGWON LEE, FAISAL SAIED, Network for Computational Nanotechnology, Purdue University, W. Lafayette, IN 47907 — The electronic structure in self-assembled quantum dots depends on the detailed quantum dot configuration inside the embedding matrix and the nearest neighbor quantum dots through electronic and strain interactions. However, realistic determination of strain requires a large computational domain. To tackle this problem for an embedded InAs quantum dot NEMO-3D uses the atomistic VFF Keating model containing up to 64 million atoms. Interatomic distance changes obtained are used to influence the sp3d5s* tight-binding electronic Hamiltonian with 21 million atoms. Targeted eigenstates with correct symmetry are found reliably even in such large systems. Our investigations show a dramatic dependence of the dot states on the size of the strain domain and the boundary conditions. NEMO-3D is also used to study the electronic states in coupled quantum dots in stacks of 2 and 7 dots. There is an interesting interplay between strain induced and size induced state distributions.

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