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Atomistic Simulation of Electronic and Optical Properties of (100), (110) and (111) Oriented InAs/GaAs Quantum Dots[1] VINAY CHIMALGI, SHAIKH AHMED, Department of Electrical and Computer Engineering, Southern Illinois University, Carbondale, IL — Recent advances in growth techniques and increasing number of experimental studies have made semiconducting InAs/GaAs quantum dots (QDs) grown along different crystallographic directions a reality and promising systems for applications in infrared detection, optical memories, laser, and in quantum cryptography as single photon sources and quantum computation. However, only few theoretical investigations have been performed on these QDs due to the complex nature of the coupling of atomicity, structural fields, polarization, and quantum size-quantization, all strong function of the crystallographic direction. The objective of this paper is to integrate a computational framework employing a combination of fully atomistic valence force-field molecular mechanics and 20-band sp^3s*d^5-SO tight-binding based electronic bandstructure models, and numerically investigate the effects of internal fields on the electronic and optical properties of InAs/GaAs quantum dots grown on (100), (110), and (111) orientated substrates. It is found that, while piezoelectricity has largest effects on lowering the symmetry of (100) oriented QDs, its effect is minimum in (111) orientated QDs.

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