Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Beyond hydrostatic strain in empirical pseudopotentials for the electronic structure of InGaAs quantum dots[1] CEYHUN BULUTAY, ASLI CAKAN, Bilkent University — Self-assembled quantum dots (SAQDs) are among the prime candidates for realizing semiconductor qubits. Even though much progress has been achieved toward understanding their electronic structure, more efforts are needed to reach the desired quantitative level for a precise control of the carrier and nuclear spin degrees of freedom. In this respect, the empirical pseudopotential method has been highly successful for structures involving more than hundred thousand atoms. However, due to lack of self-consistency, their use in strained environments, as in SAQDS, requires vital improvement. The main contribution of this work is to develop empirical pseudopotentials valid for inhomogeneous strain environments caused by cation alloying in InGaAs SAQDs. In our presentation, we first validate our approach with the ab initio density functional theory results based on Projector Augmented-Wave technique. This is followed by a comparison of the electronic structure results with and without strain-dependent pseudopotentials for InGaAs SAQDs having an alloy composition of 20-30% indium, which is typically the case in the current samples.

[1]Supported by TUBITAK with the Project No. 112T178

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Date submitted: 09 Nov 2014 Electronic form version 1.4