Comparison of the k p and direct diagonalization approaches to the electronic structure of InAs/GaAs quantum dots

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Comparison of the k·p and direct diagonalization approaches to the electronic structure of InAs/GaAs quantum dots

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We present a comparison of the 8-band **k·p** and empirical pseudopotential approaches to describing the electronic structure of pyramidal InAs/GaAs self-assembled quantum dots. We find a generally good agreement between the two methods. The most significant shortcomings found in the **k·p** calculation are i) a reduced splitting of the electron *p* states 3 vs 24 meV), ii) an incorrect in-plane polarization ratio for electron-hole dipole transitions 0.97 vs 1.24), and iii) an over confinement of both electron 48 meV) and hole states 52 meV), resulting in a band gap error of 100 meV. We introduce a ''linear combination of bulk bands'' technique which produces results similar to a full direct diagonalization pseudopotential calculation, at a cost similar to the **k·p** method. © *2000 American Institute of Physics.*_ S0003-6951 00)01903-3]

Self-assembled, Stranski–Krastanow SK) grown semiconductor quantum dots such as InAs/GaAs have recently received considerable attention.[1] They exhibit a rich spec-

examine differences in the underlying approximations of the methods. Such comparisons between **k**·**p** and pseudopotentials, using identical bulk inputs have already been performed for bulk solids,[21] superlattices,[21] and free-standing quantum dots.[17,18] The comparisons for free-standing 30–50 Å) InP,[17] CdSe,[18] and InAs[19]

tionally expensive. In this approach, we do not limit the basis to -like states Eq. 1)], but also include bulk Bloch functions, computed for a given value, , of the strain.

$$ \text{LCBB}_{i} \mathbf{r}) = \sum_{n}^{N_B} \sum_{k}^{N_k} C_{n,k}^{(i)} e^{i\mathbf{k}\cdot\mathbf{r}}] u_{n,k} , \mathbf{r}), \qquad 3) $$

where N_B and N_k are a cutoff for the number of bands and k points. The speed up of the LCBB method compared to the DD pseudopotential method arises from the fact that the LCBB states form a physically more intuitive basis than traditional plane waves and N_B and N_k can be significantly reduced to keep only the physically important bands and k points