



7 ca dUf]gcb`cZ h`Y`\_`d`UbX`X]fYWh`X]U[ cbU`nUh]cb`UddfcUW`Yg`hc`h`Y`Y`YWfcb]Wghfi`Wi`fY`  
cZ`b5g#`U5g`ei`Ubhi`a`Xchg

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# Comparison of the $\mathbf{k}\cdot\mathbf{p}$ 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  $\mathbf{k}\cdot\mathbf{p}$  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  $\mathbf{k}\cdot\mathbf{p}$  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  $\mathbf{k}\cdot\mathbf{p}$  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.<sup>1</sup> They exhibit a rich spec-

examine differences in the underlying approximations of the methods. Such comparisons between  $\mathbf{k}\cdot\mathbf{p}$  and pseudopotentials, using identical bulk inputs have already been performed for bulk solids,<sup>21</sup> superlattices,<sup>21</sup> and free-standing quantum dots.<sup>17,18</sup> The comparisons for free-standing 30–50 Å) InP,<sup>17</sup> CdSe,<sup>18</sup> and InAs<sup>19</sup>

tionally expensive. In this approach, we do not limit the basis to  $\psi_{n,k}$ -like states [Eq. 1)], but also include bulk Bloch functions, computed for a given value,  $\epsilon$ , of the strain.

$$\psi_i^{\text{LCBB}}(\mathbf{r}) = \sum_n^{N_B} \sum_k^{N_k} C_{n,k}^{(i)} e^{i\mathbf{k}\cdot\mathbf{r}} u_{n,k}(\epsilon, \mathbf{r}), \quad 3)$$

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