Comp. between 20-band TB and 8-band k.p for ZB QDs

P. Sengupta, S.Lee. S. Steiger, H. Ryu and G. Klimeck

Objective

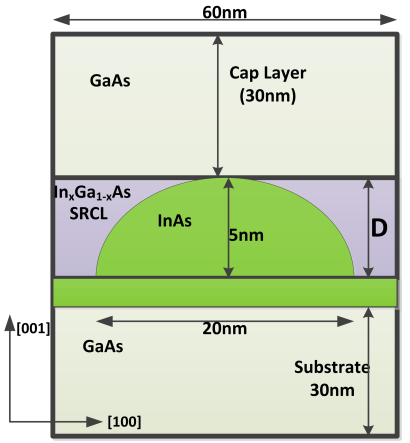
- Compare eigen values for ZB quantum dots with 20-band TB and 8-band k.p

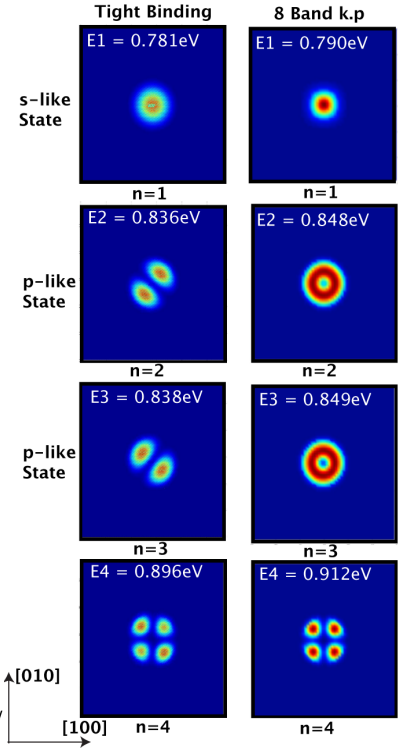
Method

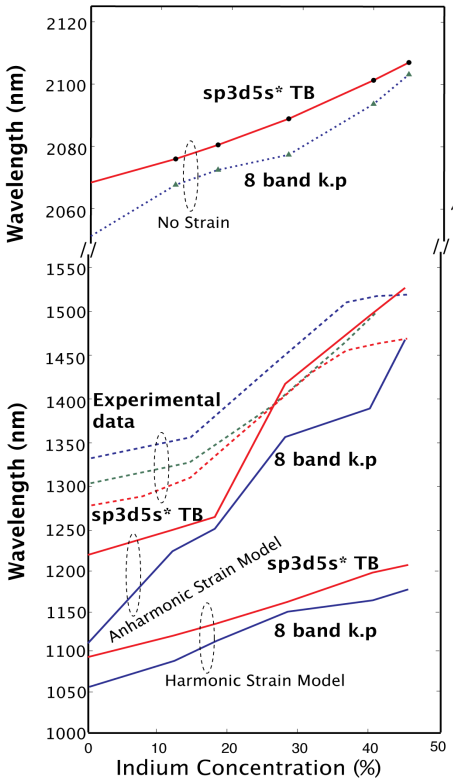
- 20-band TB with Valence Force Field (VFF) strain calculations
- 8-band k.p calculations with finite-difference discretization
- Strain computed by interpolating atomic VFF results on continuum grid and traditional continuum elastic model

Results

- Eigen values from TB and k.p reasonably matched
- Wave-function for n=2,3 different in TB from k.p
- Eigen values are better matched to experimental results with anharmonic VFF







Multiscale approach (atomistic strain + continuum electronic structure) is roughly 6-times faster than atomistic approach