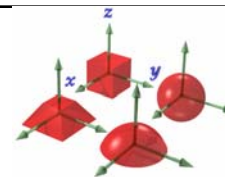


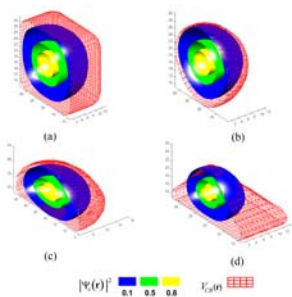
3D Quantum Dot Interdiffusion Model

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Objective: to develop a three dimensional modeling tool for epitaxial growth and postgrowth bandgap engineering process of quantum-dot (QD) and interdiffused QDs.



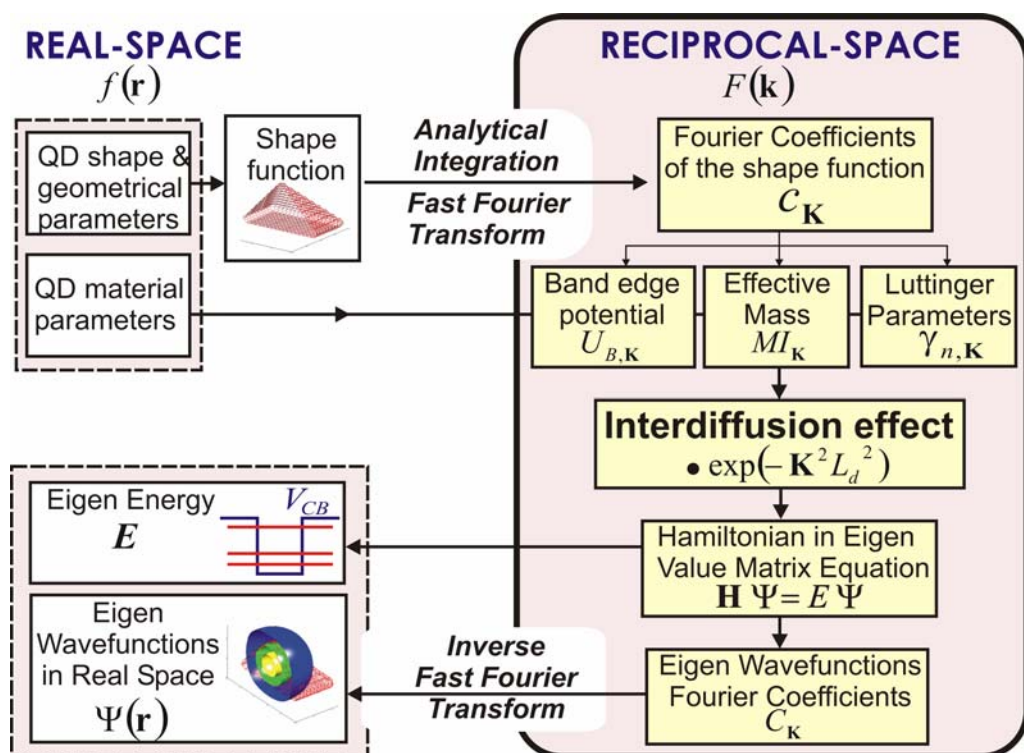
Novel idea for 3D interdiffused QD model:

- Hamiltonian in the reciprocal space domain
 - Applied to calculate electronic structure of cubical, spherical, lens-shaped, pyramidal QDs.
- a discrete function in reciprocal space \rightarrow a periodic function in real space

Advantages:

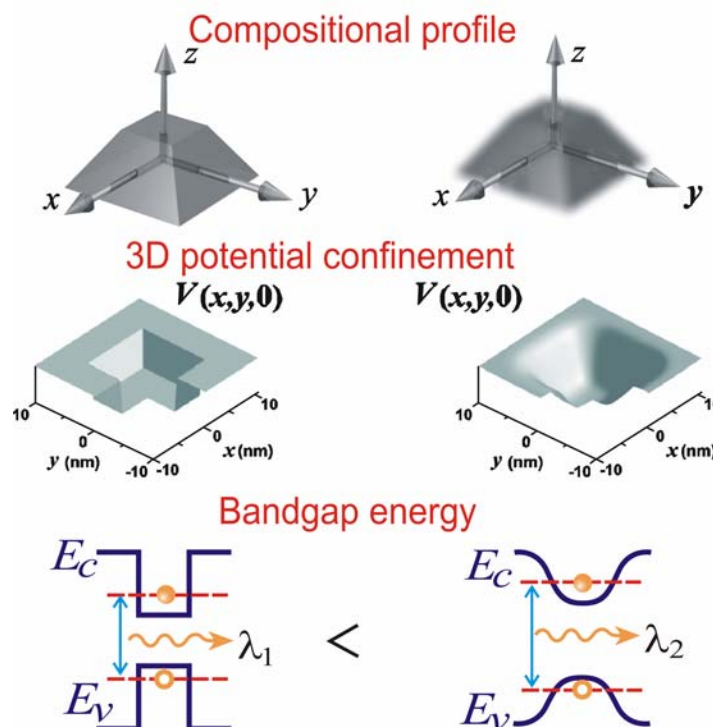
1. Significantly reduce the matrix size of Hamiltonian
2. Natural solution to the diffusion equation
3. Natural representation of QDs arrays
4. Applicable to complex interdiffused QD structures such as QD+wetting layer, dot-in-well, InAs/GaAs columnar QDs.

Model Flowchart:

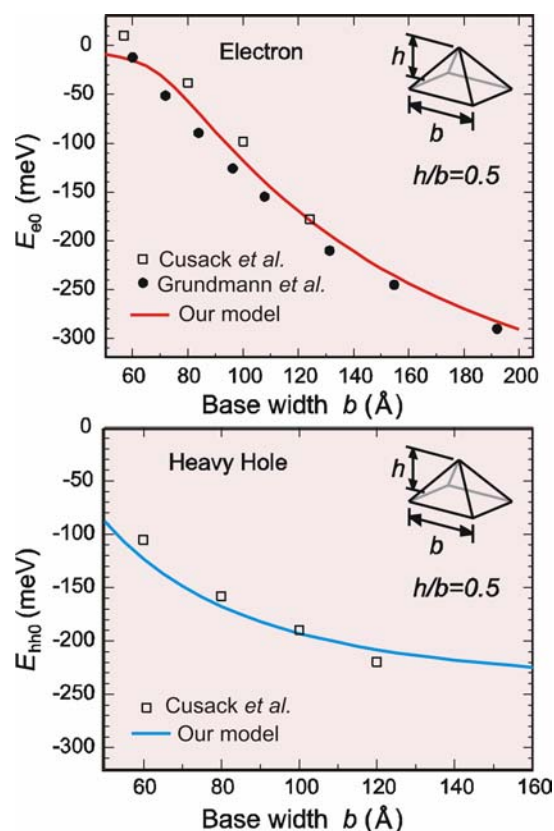


Before interdiffusion:

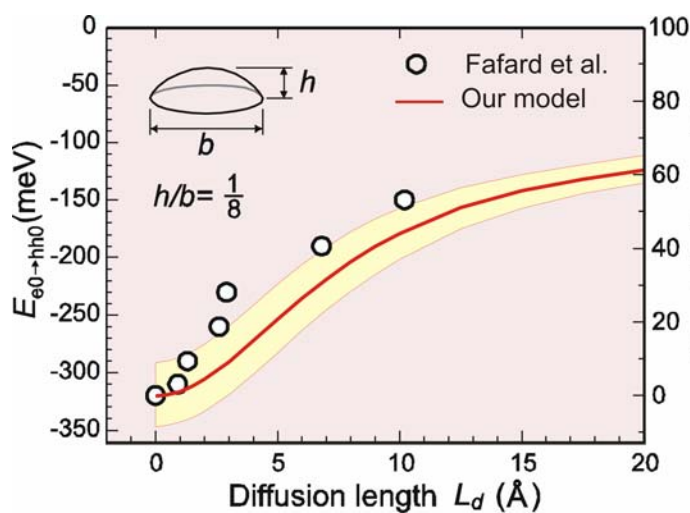
After interdiffusion:



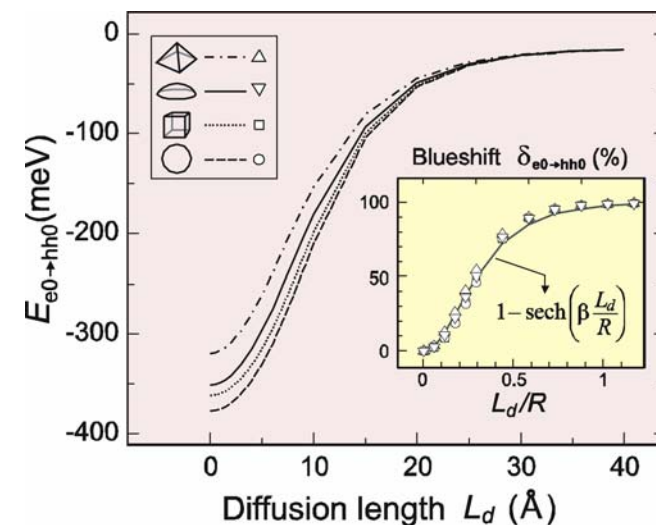
Verification with other models:



Verification with the experimental data of interdiffused QD:



Sech rule for general interdiffused QD:



Without considering the interdiffusion effect ($L_d=0\text{\AA}$), we reproduce the more complicated calculation results from Cusack et al. [1] and Grundmann et al. [2].

Using the experimental data from Fafard et al. [3], our model yields a reasonably good agreement for the interdiffused lens-shaped QDs.

We found similar blueshift profile in different QD shapes (spherical, cubical, pyramidal and lens-shaped) at almost any size that can be well approximated by sech(x) function.

Ref: ¹M. A. Cusack, P. R. Briddon, and M. Jaros, *Phys. Rev. B* 54, R2300 (1996)
²M. Grundmann, O. Stier, and D. Bimberg, *Phys. Rev. B* 52, 11969 (1995).
³S. Fafard and C. N. Allen, *Appl. Phys. Lett.* 75, 2374 (1999).