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Impact of charged defects on silicon MOS quantum dots

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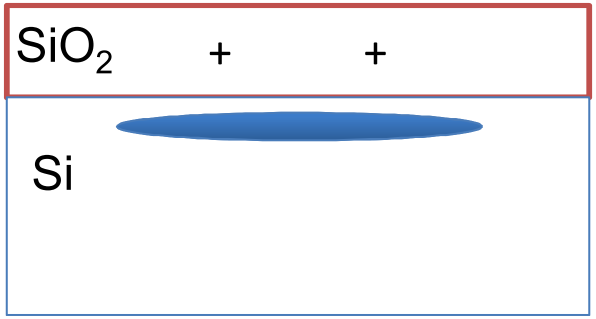
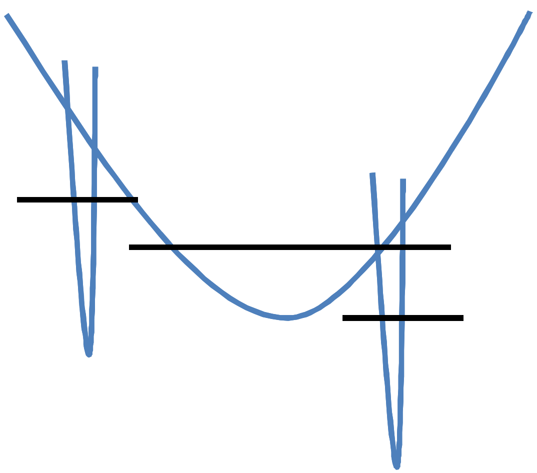
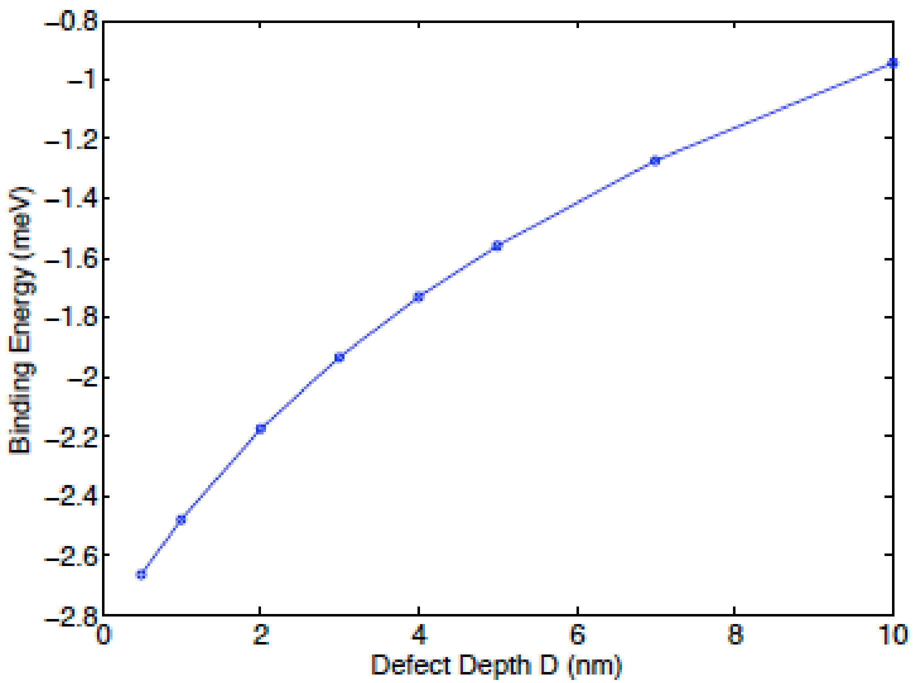
Charge Defects in SiO_2



Schematic of potential

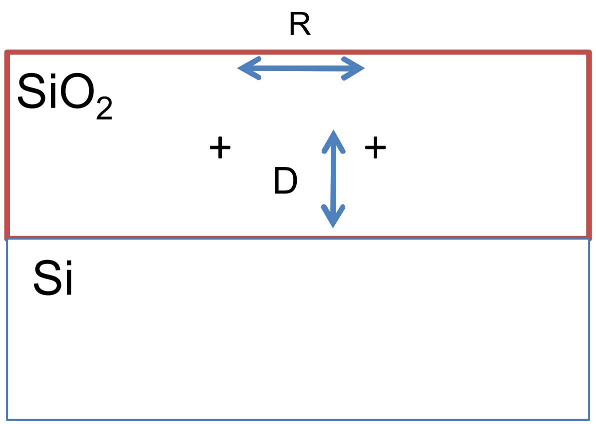


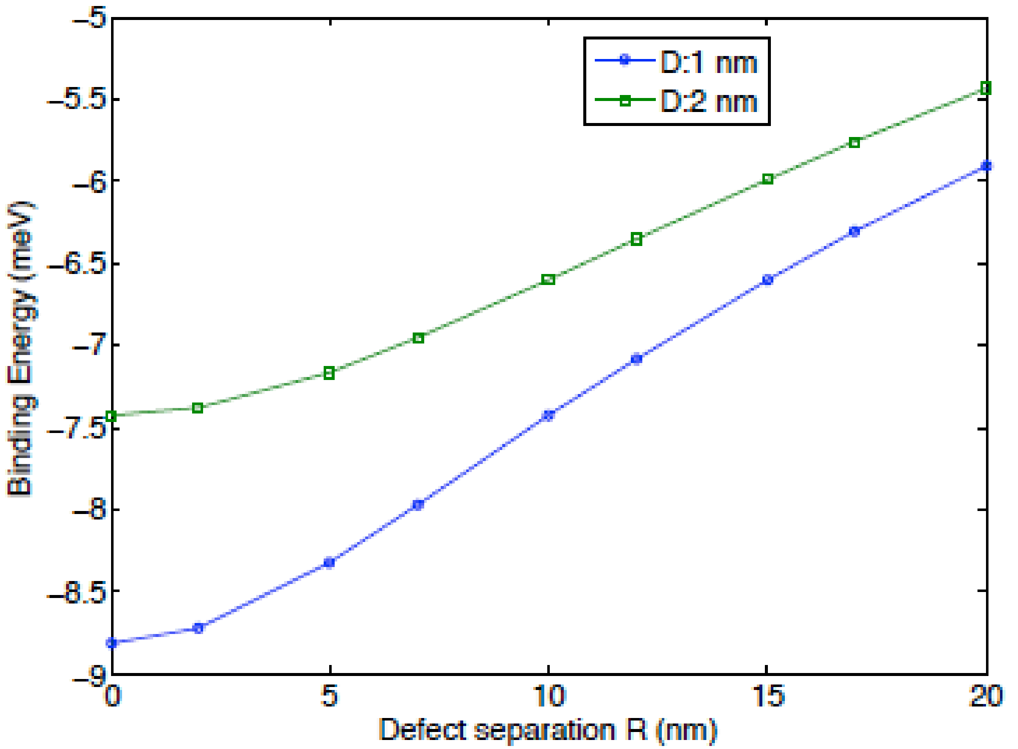
Tight-binding calculation of energy levels of a single defect



Cluster of Defects

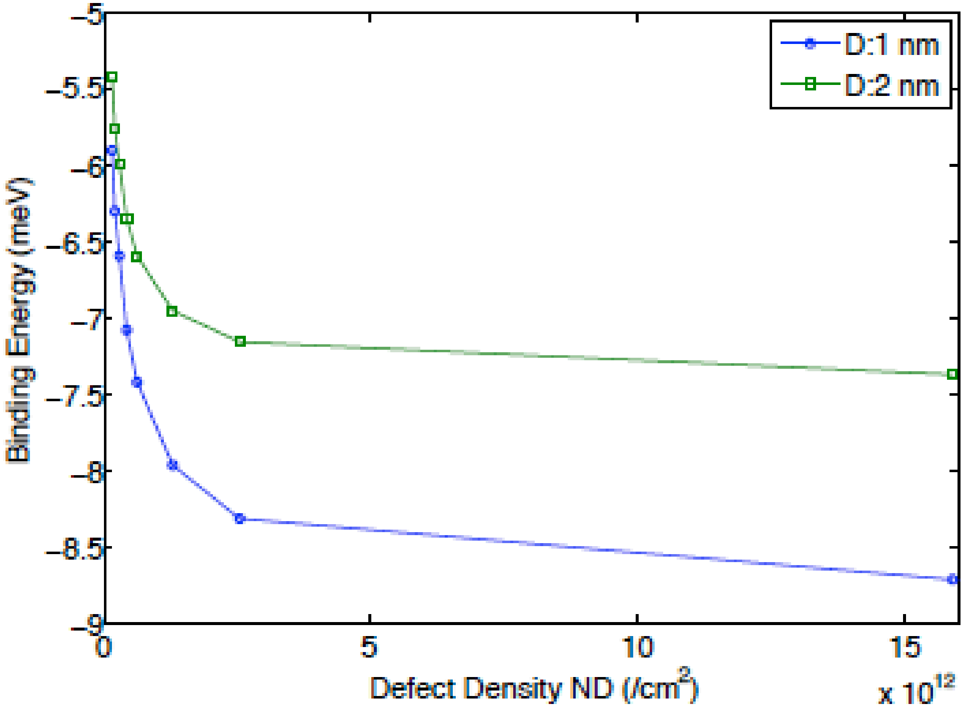
TB calculations of defect levels vs R for 2 depths



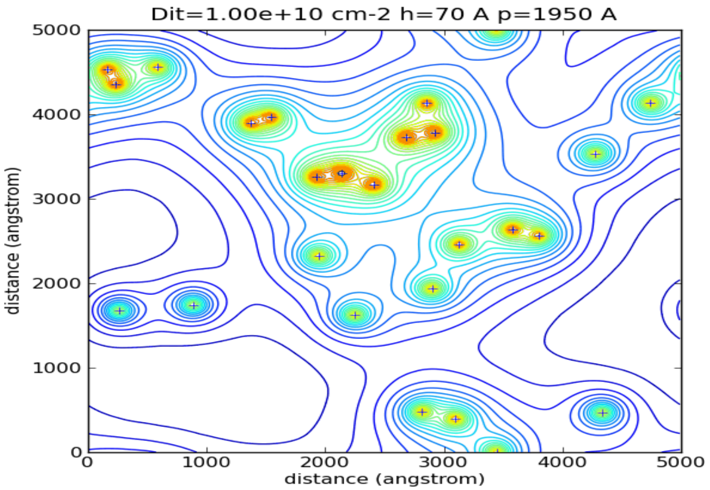


Cluster of Defects

Binding energy vs defect density



Puddles of electrons



Goal: DQD J-curve in the presence of charge defects

Good 1e wfs + Full CI for few electrons

Atomistic tight-binding (NEMO 3D)

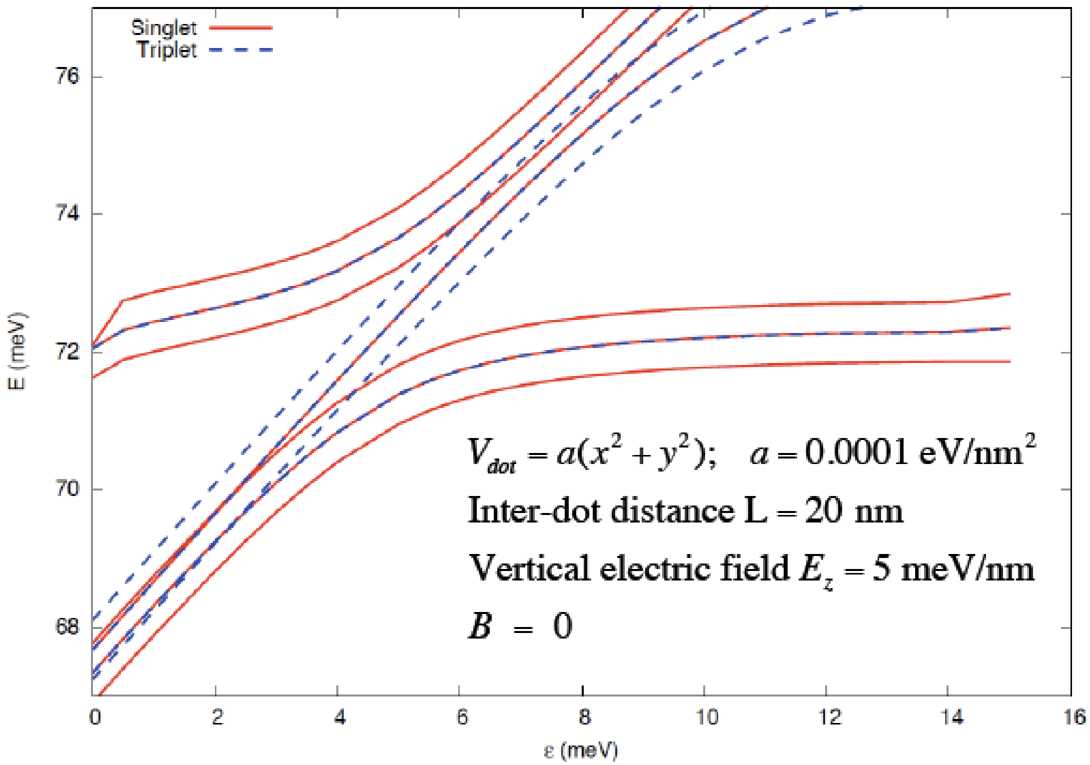
- LCAO, full bandstructure method (no extra parameter for VS)
- miscut (tilt)
- surface roughness
- alloy disorder
- strain
- hetero-structures
- realistic device geometries
- E-fields
- B-fields
- multi-million atom systems (HPC)

Configuration Interaction
E. Nielsen, et. al. PRB 82, 075319 (2010).

- Few electron full Hamiltonian
- J, K in k-space
- Computational speed (HPC)

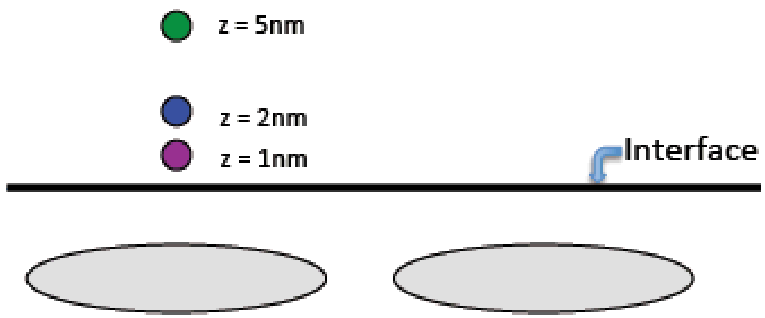
2e states of an ideal DQD

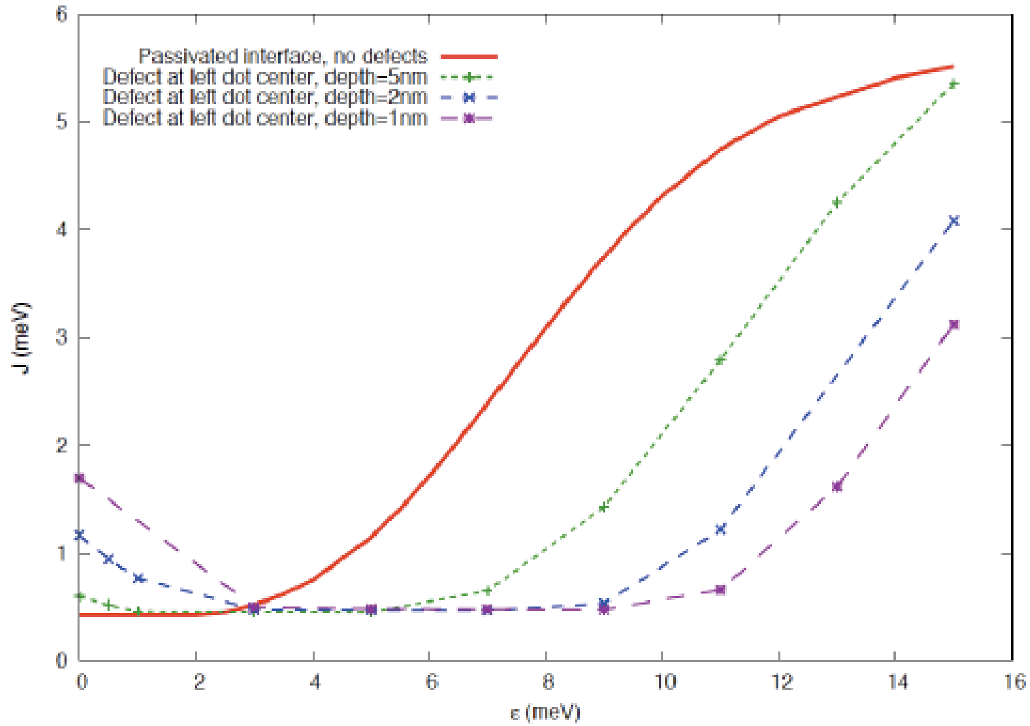
Total Energies: Ideal DQD (with valleys)



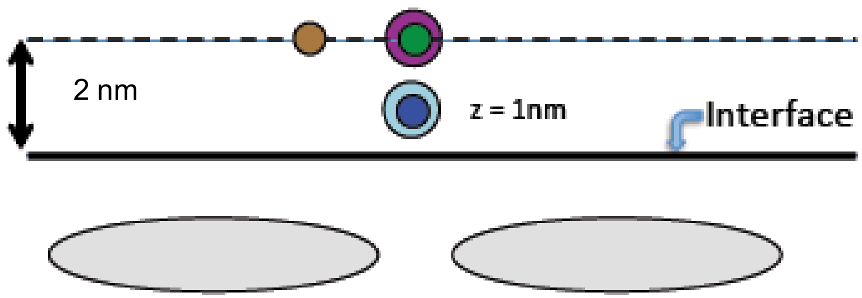
Ideal J-curve

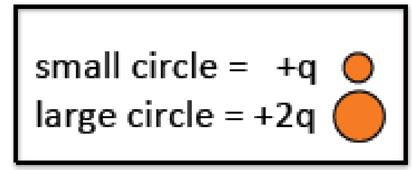
Defect at dot center

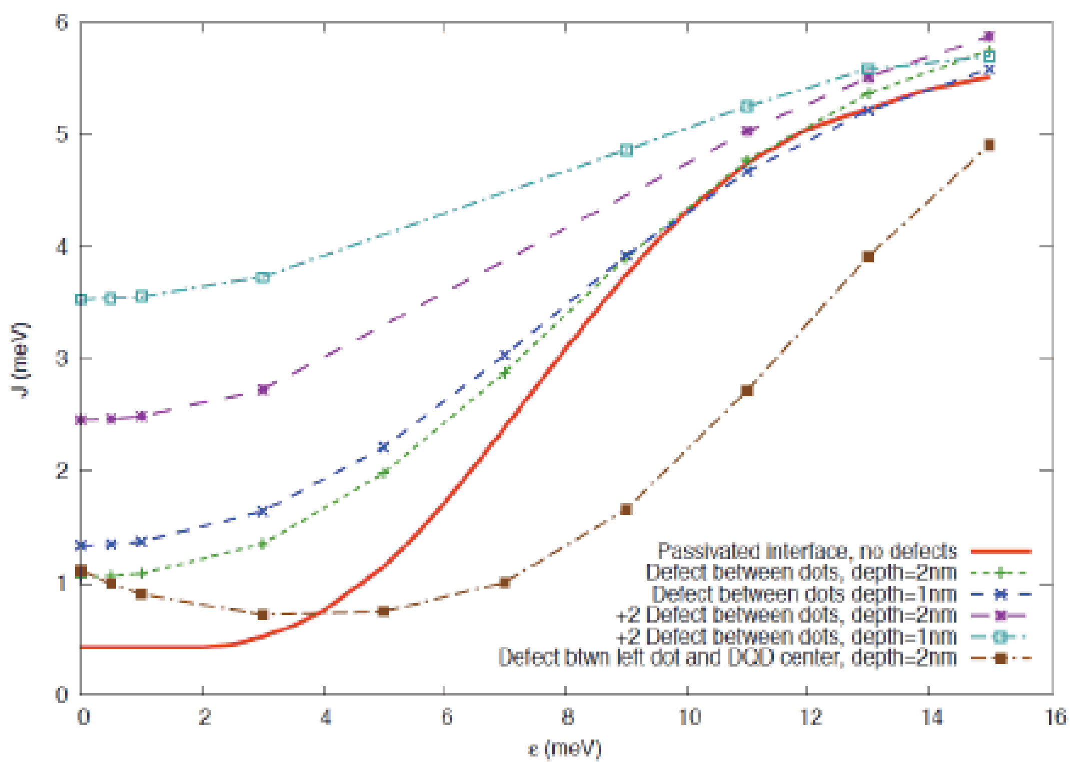




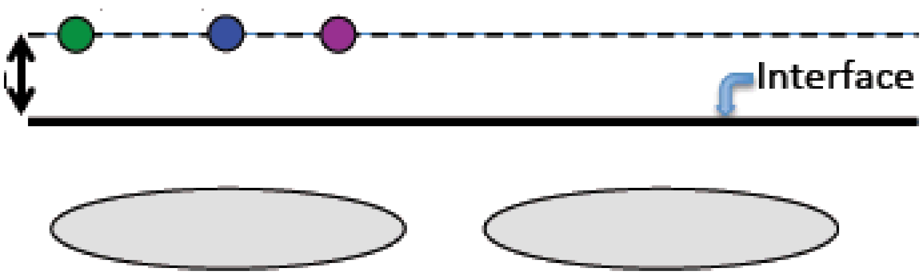
Defect at tunnel barrier between dots

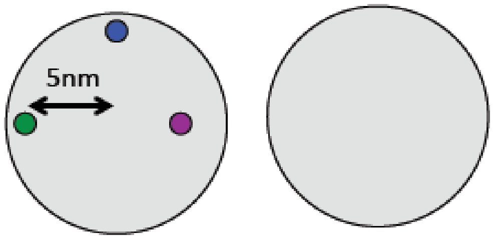


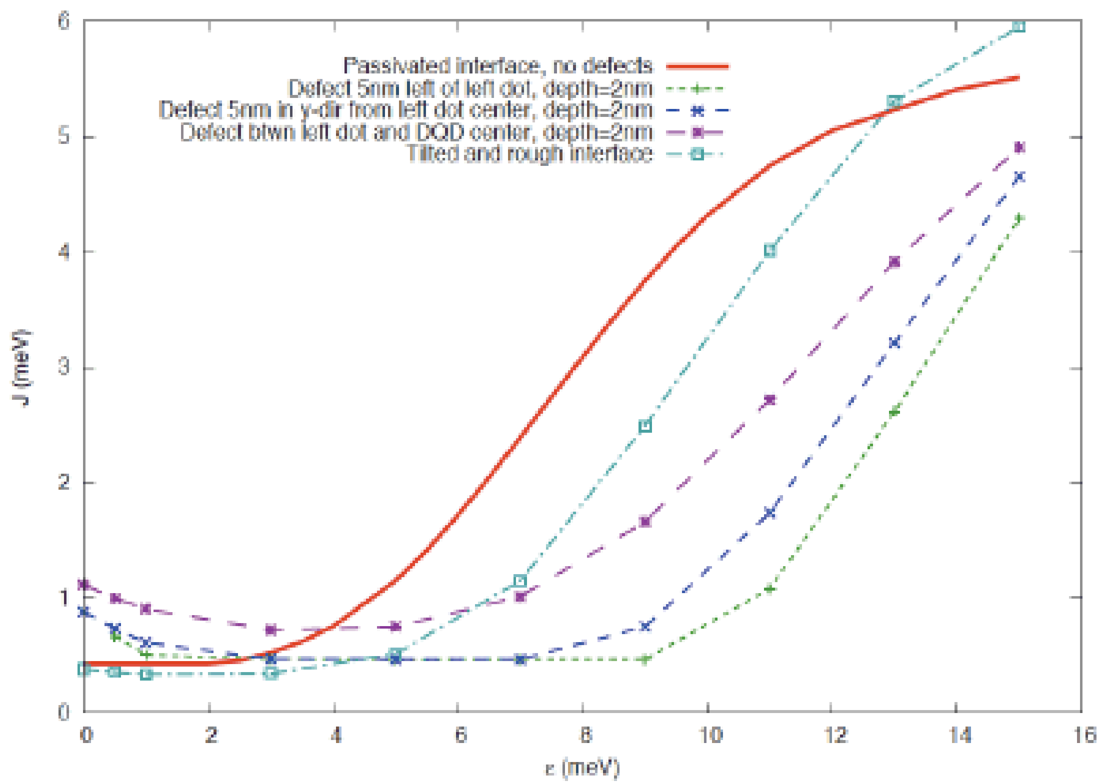




Defect at different distances from barrier







Conclusions

- Single and multiple charge defects can bind electrons below the CB
- Defects cause perturbations in the SQD and DQD potential
- Developed TB + CI methodology to investigate J-curves
- J-curves are sensitive to defect locations and densities