

Objective:

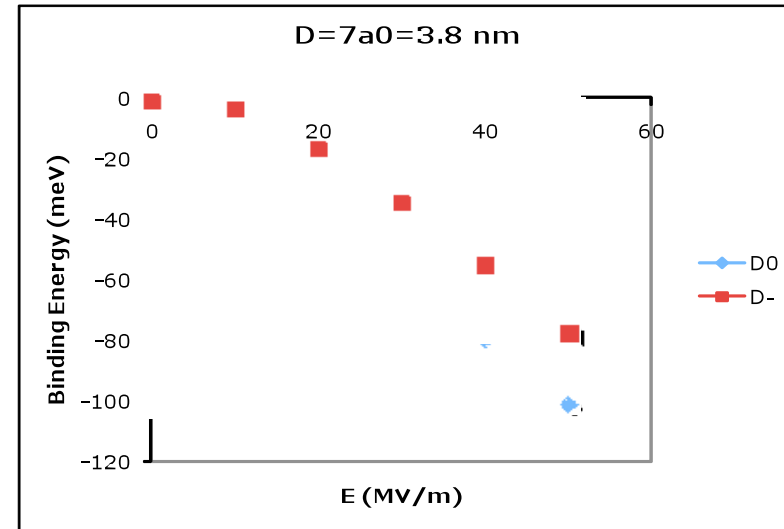
- Obtain two electron binding energy for Group V donors as a function of E-fields and donor depths.
- D- ground and excited states: Analyze measured Coulomb diamonds from Transport Spectroscopy measurements.

Approach:

- Use a domain of 1.4 M atoms with 1 donor.
- 1st approximation: SCF Hartree method.
- 2nd SCF: 1. Obtain wf from NEMO
2. Calculate electron density and Coulomb repulsion potential
3. Repeat NEMO simulation with the new potential.
- 4. Break when D- energy has converged.
- 3rd: On-going: D- from configuration interaction

Results:

- In the Hartree approximation, D- energy for a bulk donor varies by about 2 meV from measured value.
- D- with field (0 to 50 MV/m) for a donor 3.8 nm from interface.
- Next step : Model interface screening.



E (MV/m)	0	10	20	30	40	50
D- (meV)	-0.90	-3.78	-16.62	-34.47	-54.89	-77.08
	2.78	-0.52	-13.94	-31.82	-51.71	-73.07
	4.58	6.13	-5.73	-21.35	-45.69	-68.37
D0 (meV)	-52.49	-52.53	-54.82	-62.26	-79.45	-100.83
	-32.31	-34.71	-39.19	-58.15	-76.37	-96.99
	-26.66	-30.65	-43.52	-50.77	-59.01	-84.78