ICSS 2016

INTERFACE EFFECTS ON ACCEPTOR SILICON QUBITS

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OVERVIEW

- 1. INTRODUCTION.
  - Quantum computing.
  - Silicon QC. Kane proposal with donors.
  - Acceptor based QC.
- 2. PROBLEM: ACCEPTORS NEAR AN INTERFACE
- 3. RESULTS

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BUILDING A QUANTUM COMPUTER

- Why build a QC?
  - Information security. Shor algorithm for prime factorization. Quantum cryptography.
  - Database search. Grover algorithm.
  - Quantum simulations.

BUILDING A QUANTUM COMPUTER

- QC proposals
  - Ion traps
  - NMR
  - Topological states
  - Electron spin in SC (Si, Ge, GaAs…)
  - NV centers
  - Josephson junctions
  - Photon polarization
  - Nuclear spin in SC (Si)

WHY SILICON?

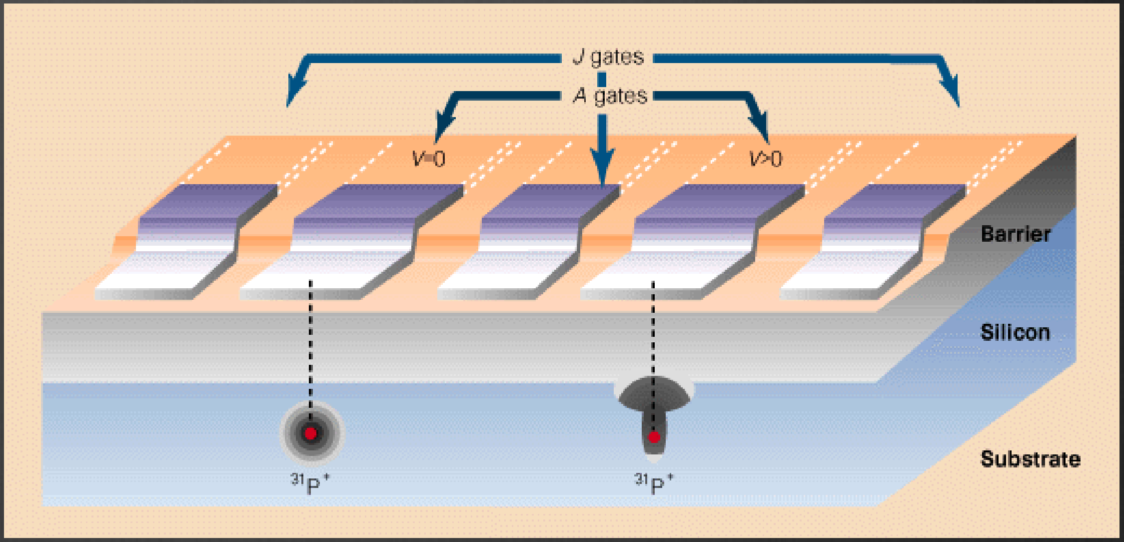
- Ideal environment for spin qubits. Weak SO-coupling and isotopes with zero nuclear spin.
  - Spin coherence times > 30s (Phosphorus nucleus). J. Muhonen et. al., Nature Nanotechnology, 9, 986 (2014)
- Availability of the state-of-the-art crystal growth, processing, isotope engineering technologies and well known physical properties
- Possible integration with 'classical' Si devices

Dopant-based silicon QC

B.E.Kane, Nature 393, 133 (1998);
Fortschr. Phys. 48, 9 (2000)

Building block is the donor electron-nucleus system

- P donors in Si: nuclear spin ½
- Electron spin coupled to nuclear spin by hyperfine interaction

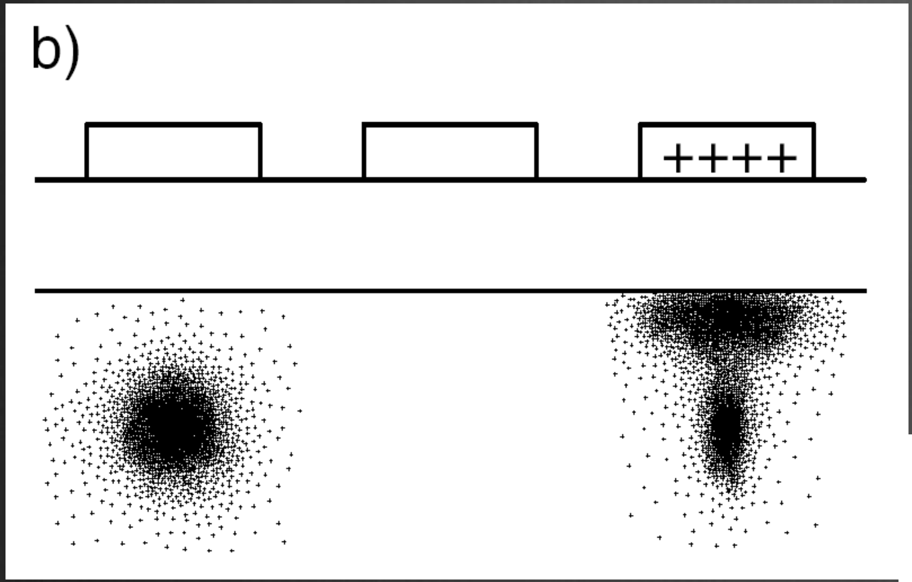


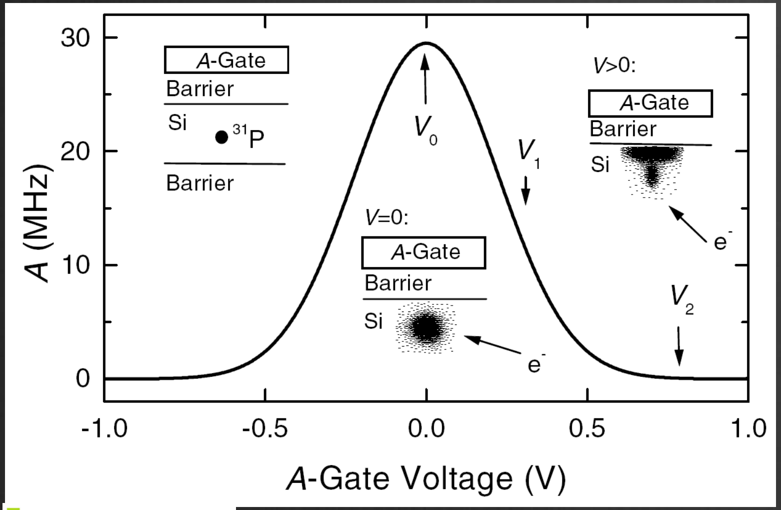
- A gate controls the hyperfine interaction
- J gate controls the overlap of electrons
- Readout: Spin-dependent tunneling

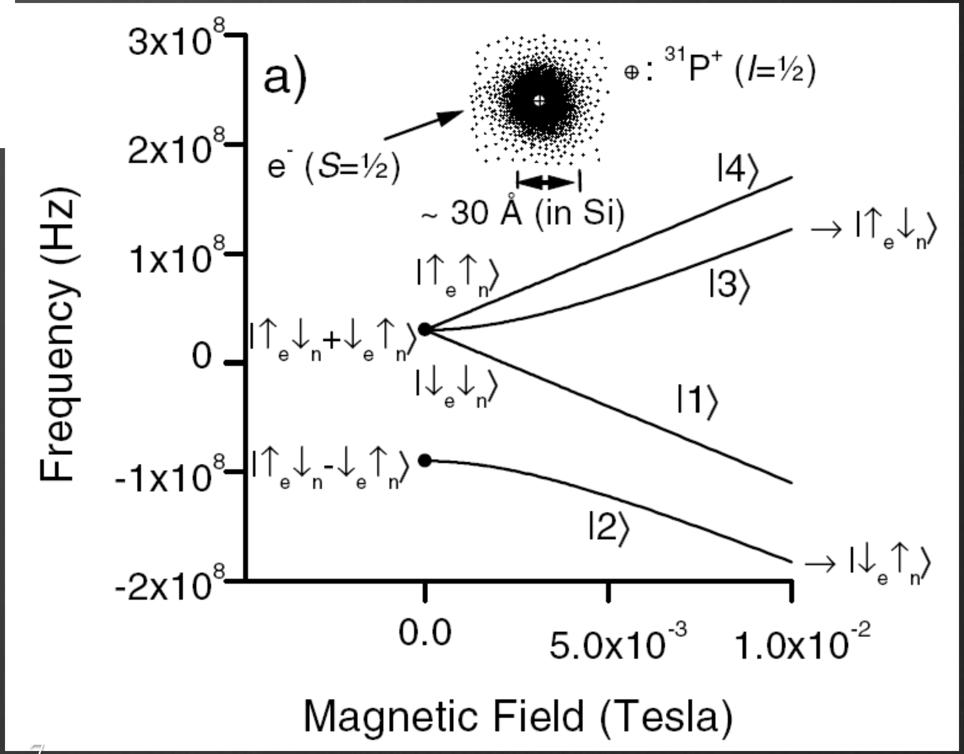
Logic operations in Si:^{31}P – 1 qubit operations

$$H = 2\mu_B B\sigma_z^e - g_n\mu_n B\sigma_z^n + A\sigma^e\cdot\sigma^n$$

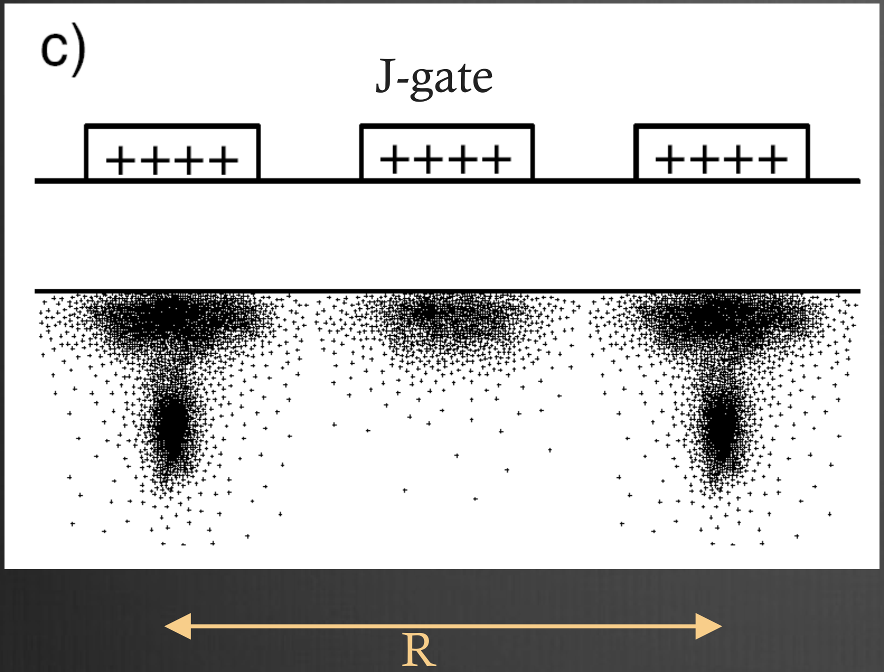
$$A = \frac{4}{3}\pi g_e\mu_B g_n\mu_n\left|\Psi(0)\right|^2$$







Logic operations in Si:^{31}P – 2 qubit operations



$$H_\sigma = J(R)\sigma^{1e} \cdot \sigma^{2e}$$

EXCHANGE

$$U_\sigma(t) = T\exp\left\{-i\int_0^t H_\sigma(t')dt'\right\}$$

Pulse duration τ_σ:

$$\int dt\, J(t) = J_0\tau_\sigma = \pi \bmod(2\pi)$$

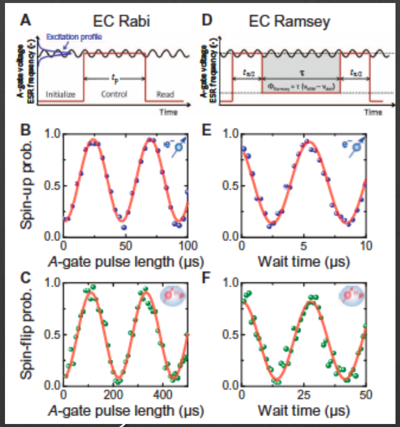
a 'swap' occurs

$$U_{CNOT} = exp(i(\pi/2)\sigma_1^z)exp(-i(\pi/2)\sigma_2^z)U_\sigma^{1/2}(\tau_\sigma)exp(i(\pi/2)\sigma_1^z)U_\sigma^{1/2}(\tau_\sigma)$$

Loss & DiVincenzo PRA (1998)
Kane Nature (1998)

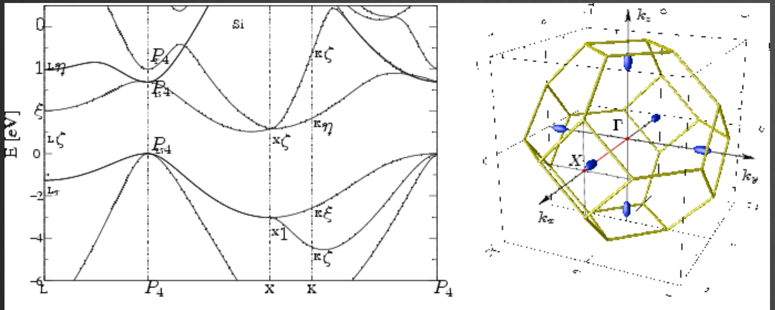
Experimental status

- High fidelity single shot readout of electron and nuclear spin. Pla et al., Nature 489, 541 (2012). J. Pla et al., Nature 496, 334 (2013)
- Electron spin relaxation and coherence times > T_1 in the order of hundreds of seconds. T_2= 10s. Nature Materials 11, 143-147 (2012)
- Nuclear spin coherence times > 30 s. Nature Nanotechnology 9, 986 (2014)
- A-gate implementation. Laucht et al. *Science Advances* Vol. 1, no. 3, e1500022 (2015)
- Fidelities above 99.9% for single and two-qubit operations (Electron and nucleus spins). J. Phys: Condens. Matter 27, 154205 (2015)

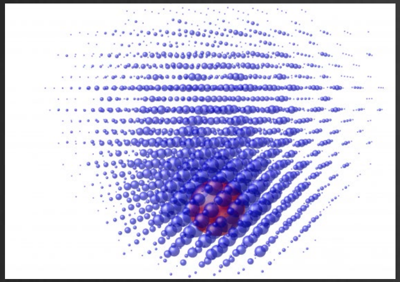


Problems with donors

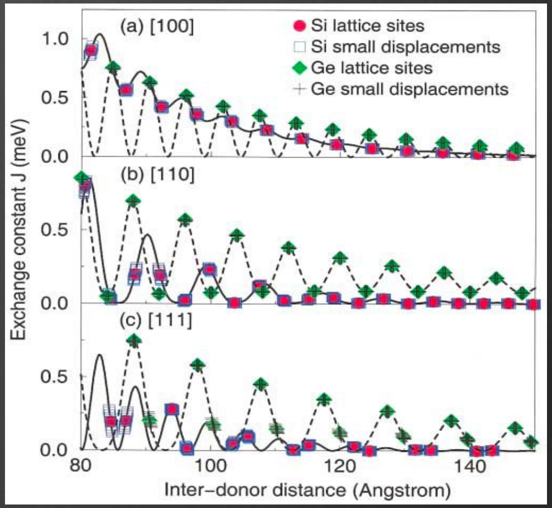
- Valley degeneracy. Exchange oscillations. Koiller et al., **PRL 88, 027903**



(a) Band diagram of silicon, (b) First conduction band valleys,



Small coupling to electric fields

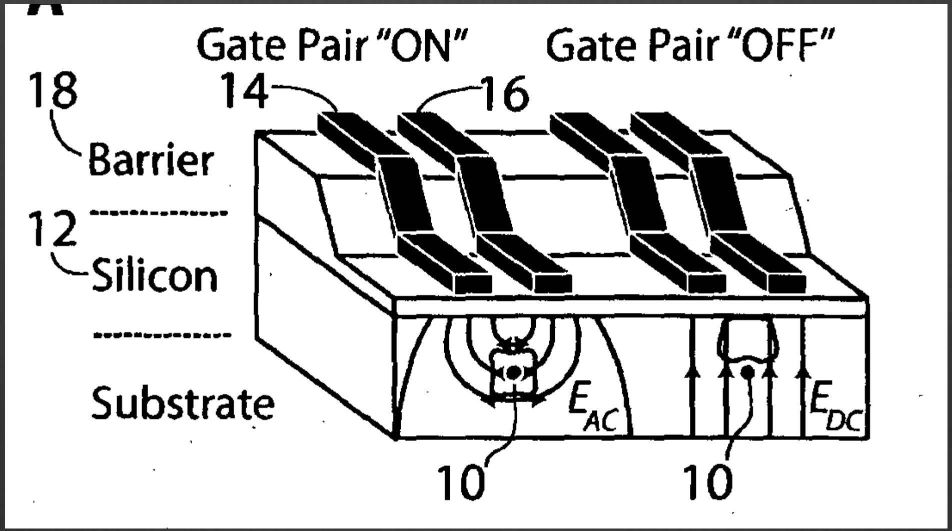


ACCEPTOR BASED QUBITS

- No valley degree of freedom.
- Exploit long range dipolar inter-qubit coupling, Golding and Dykman, cond-mat/0309147.
- Exploit spin-orbit interaction (however, SO is also a cause of decoherence)
  - Couple spins to phonons, Ruskov and Tahan, PRB 88, 064308 (2013).
  - Couple spins to oscillating electric fields, Salfi et al PRL 116, 246801.

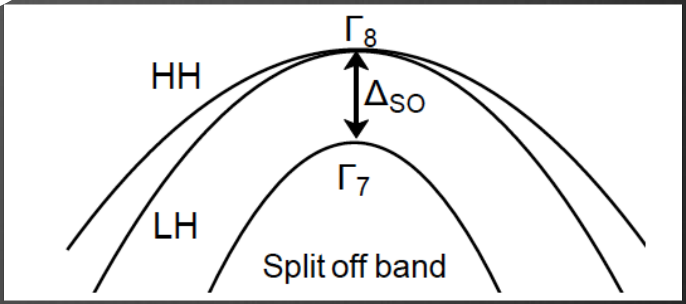
ACCEPTOR BASED QC

- Gate pair controls a single acceptor
- Exchange gate or dipolar coupling for acceptor-acceptor interaction

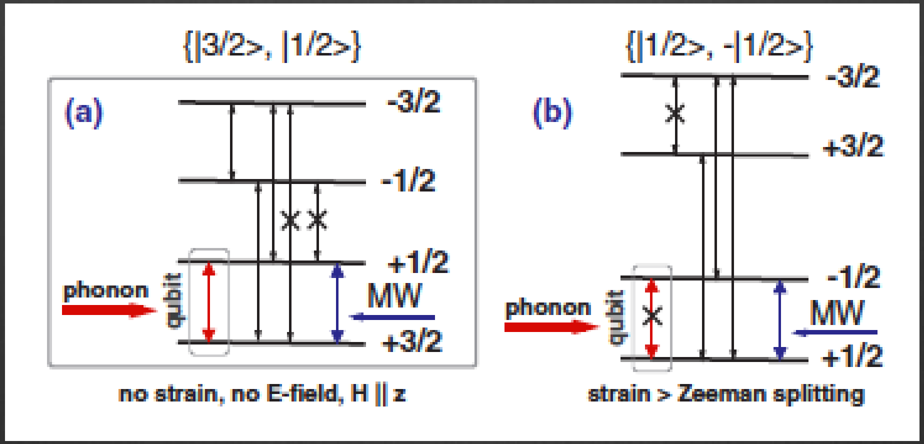


- Rogge et al., Patent PCT/AU2014/000003

ACCEPTOR BASED QC

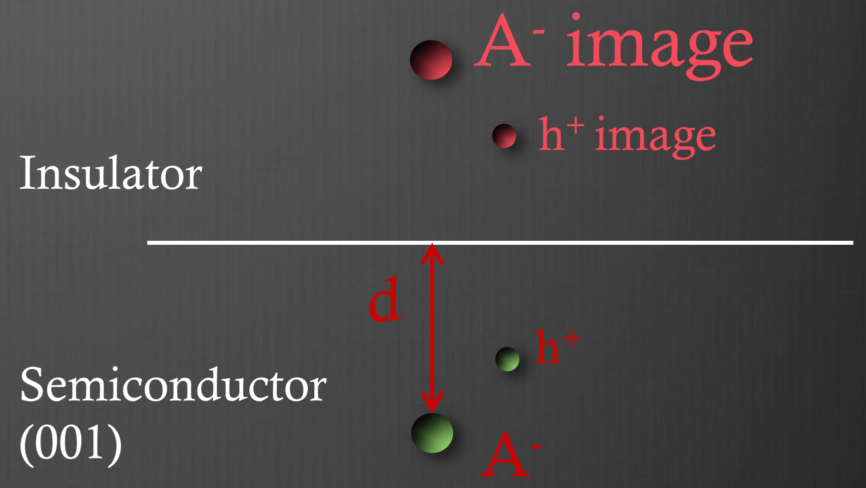


- Acceptor GS is 4-fold degenerate (J=3/2)
- Quantum confinement, strain and E fields partially lift the degeneracy
- Magnetic fields removes degeneracy



Ruskov and Tahan: Phys. Rev. B 88, 064308

FOCUS



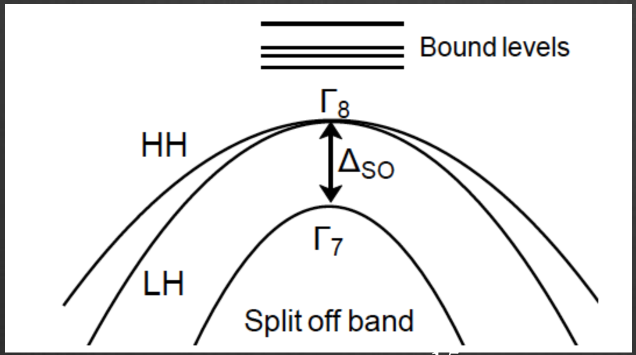
How are acceptor bound states affected by the proximity of an interface?

- Binding energies
- Symmetries

KOHN-LUTTINGER HAMILTONIAN

$$Ry^*(Si) = 24.8\, meV$$
$$a^*(Si) = 2.55\, nm$$
$$Ry^*(Ge) = 4.4\, meV$$
$$a^*(Ge) = 10.85\, nm$$

$$H_{\mathrm{KL}} = \begin{pmatrix} P+Q & L & M & 0 & \frac{i}{\sqrt{2}}L & -i\sqrt{2}M \\ L^* & P-Q & 0 & M & -i\sqrt{2}Q & i\sqrt{\frac{3}{2}}L \\ M^* & 0 & P-Q & -L & -i\sqrt{\frac{3}{2}}L^* & -i\sqrt{2}Q \\ 0 & M^* & -L^* & P+Q & -i\sqrt{2}M^* & -\frac{i}{\sqrt{2}}L^* \\ -i\sqrt{2}L^* & i\sqrt{2}Q & i\sqrt{\frac{3}{2}}L & i\sqrt{2}M & P+\Delta_{SO} & 0 \\ i\sqrt{2}M^* & -i\sqrt{\frac{3}{2}}L^* & i\sqrt{2}Q & i\sqrt{2}L & 0 & P+\Delta_{SO} \end{pmatrix}$$



$$P = -\mathbf{k}^2 + \frac{2}{r}$$
$$Q = -\frac{\gamma_2}{\gamma_1}(k_x^2 + k_y^2 - 2k_z^2)$$
$$L = i2\sqrt{3}\frac{\gamma_3}{\gamma_1}(k_x - ik_y)k_z$$
$$M = -\sqrt{3}\frac{\gamma_2}{\gamma_1}(k_x^2 - k_y^2) + i2\sqrt{3}\frac{\gamma_3}{\gamma_1}k_x k_y$$

ACCEPTOR CLOSE TO AN INTERFACE

$$H_{\text{acceptor}} = H_{\text{KL}} + V_{\text{cc}}(r) + V_{ic}(\rho, z)$$

Central cell correction:

$$V_{\text{cc}} = \frac{2(\epsilon_s - 1)e^{-r/r_{\text{cc}}}}{r}$$

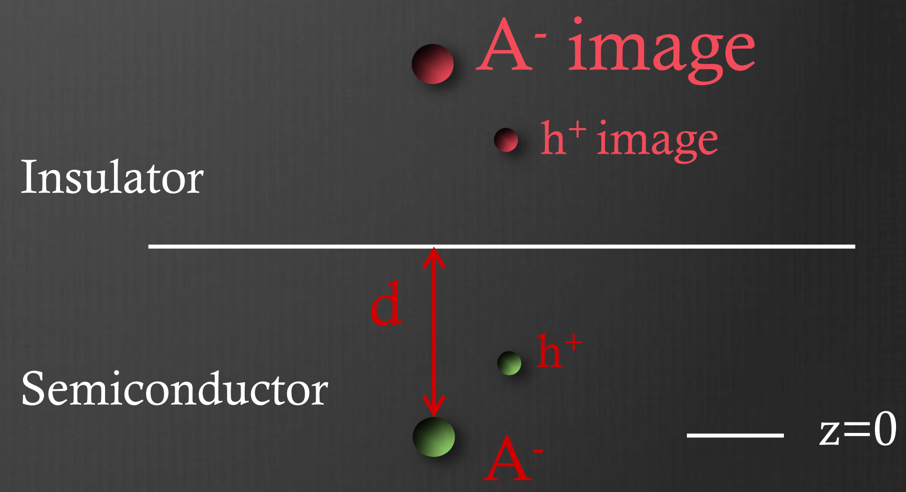


Image charges:

$$V_{ic}(\rho, z) = -\frac{2Q'}{\sqrt{\rho^2 + (z+2d)^2}} + \frac{Q'}{2(z+d)}$$

$$Q' = \frac{\epsilon_b - \epsilon_s}{\epsilon_b + \epsilon_s}$$

Assume a hard wall boundary condition at z=-d

VARIATIONAL BASIS SET

$$\psi(\rho, z, \varphi, \alpha_i) = (z+d) z^{l'} \rho^{|L_z|} r^{n'} e^{-\alpha_i r + i L_z \varphi} |J, J_z\rangle$$

cylindrical variables

Hard-wall

l'=L-|L_z|

n'=n-L-1, n>L

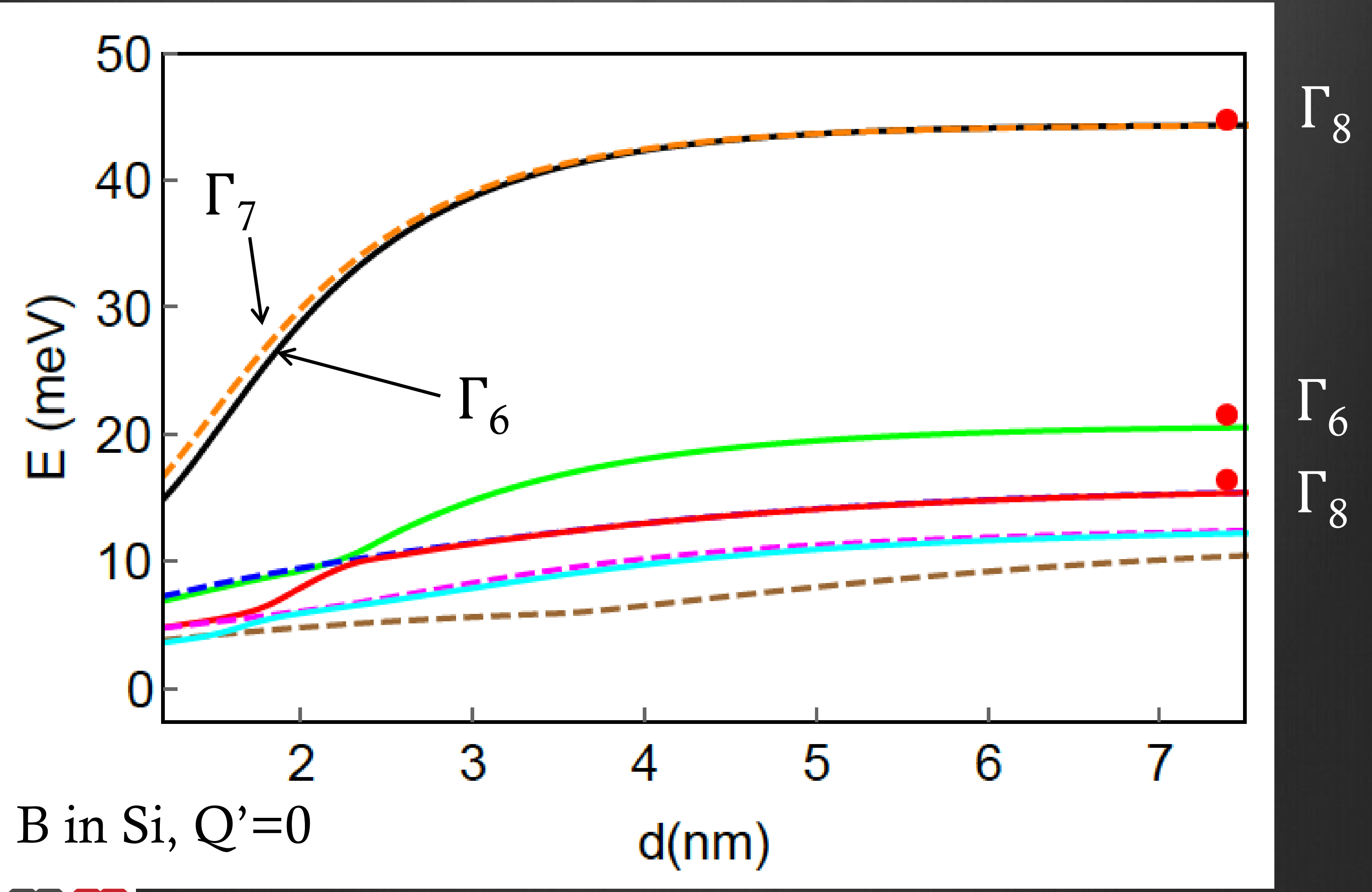
set of values, i≤4

IR	Degeneracy	$F_z=J_z+L_z$
Γ_6	2	±1/2+4n
Γ_7	2	±3/2+4n
Γ_8	4	any half integer

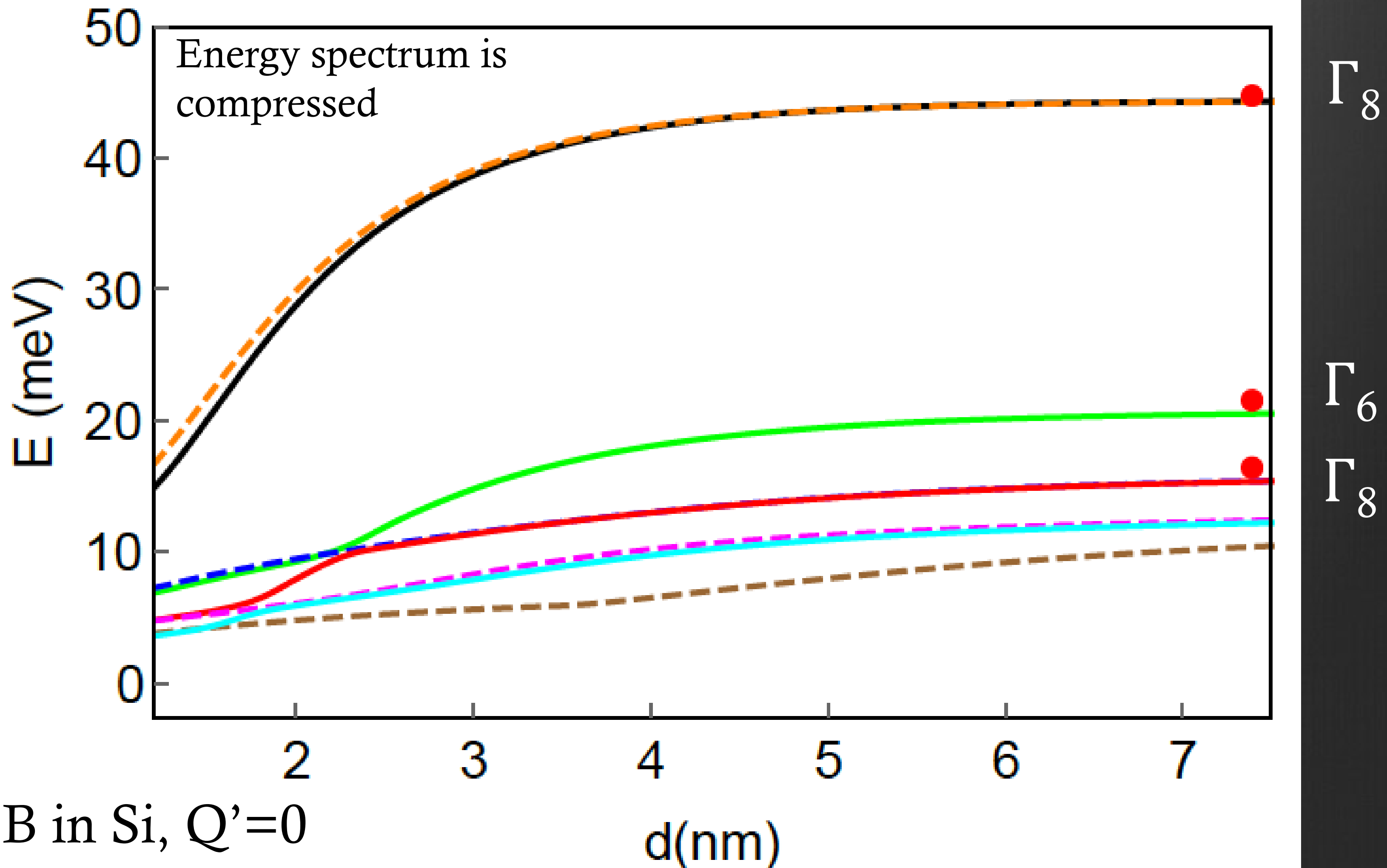
The interface reduces the symmetry and Γ_8 becomes a reducible representation:

$\Gamma_8=\Gamma_6\oplus\Gamma_7$

RESULTS: ENERGY SPECTRUM

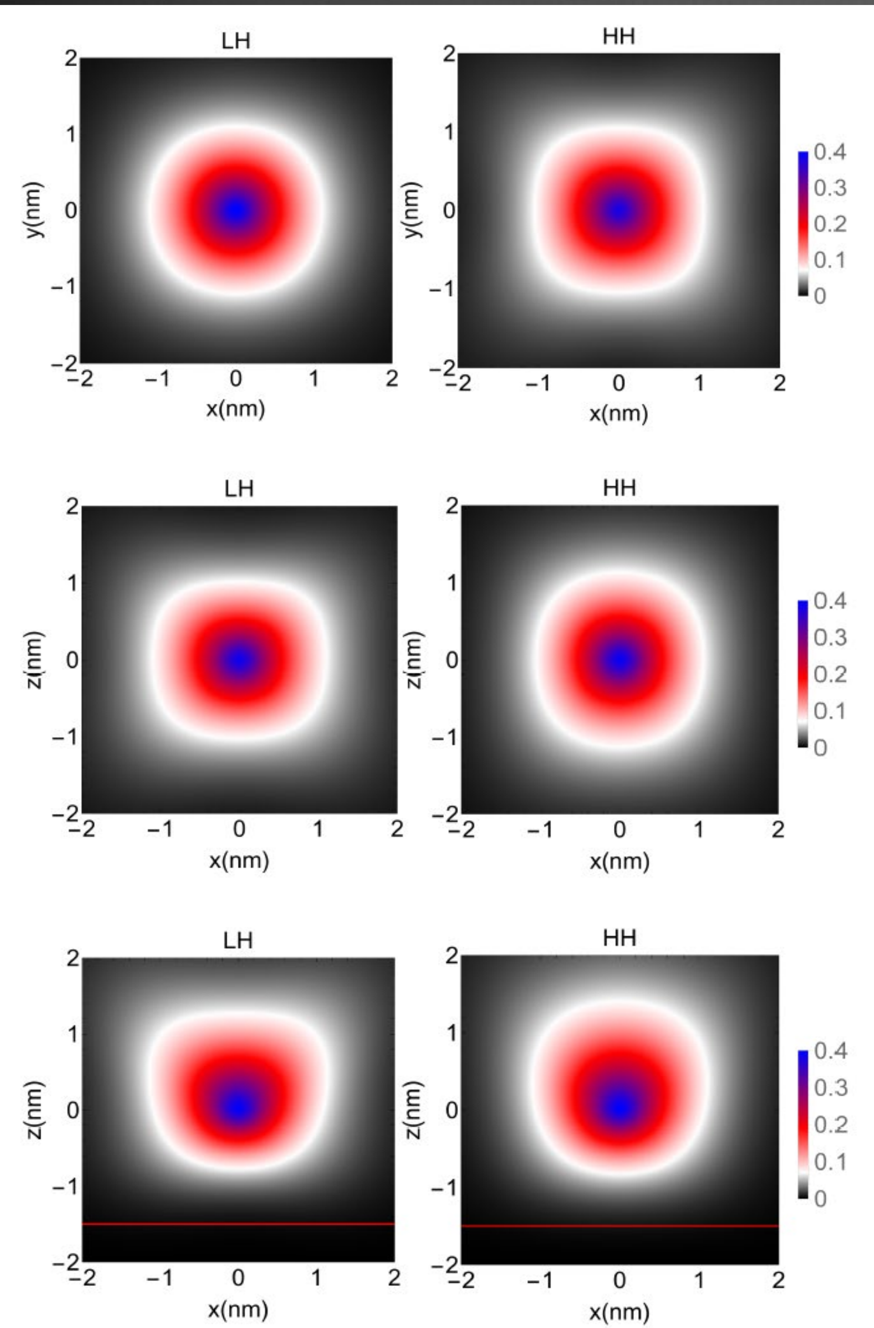


RESULTS: ENERGY SPECTRUM



B in Si, Q'=0

Γ_6 Γ_7



GROUND STATE WAVE-FUNCTIONS

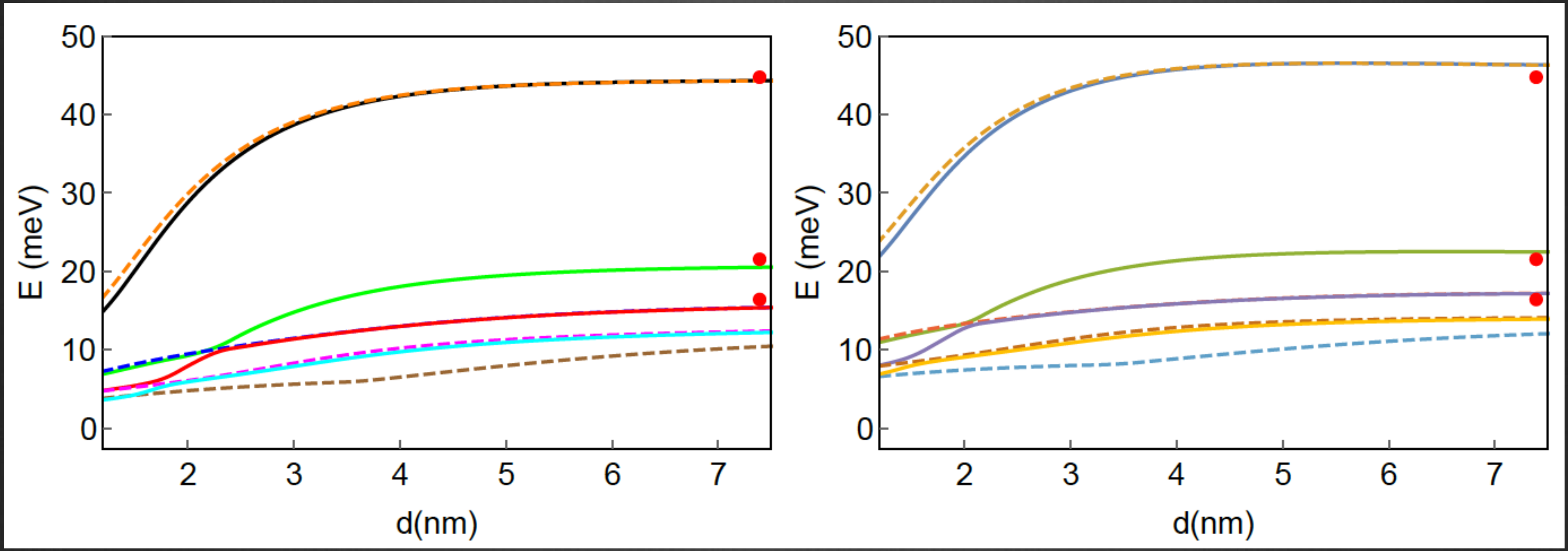
d=2 nm
Parallel to interface

d=7.5 nm

Different shapes of the wave-funtions lead to the ground state energy splitting.

d=1.5 nm

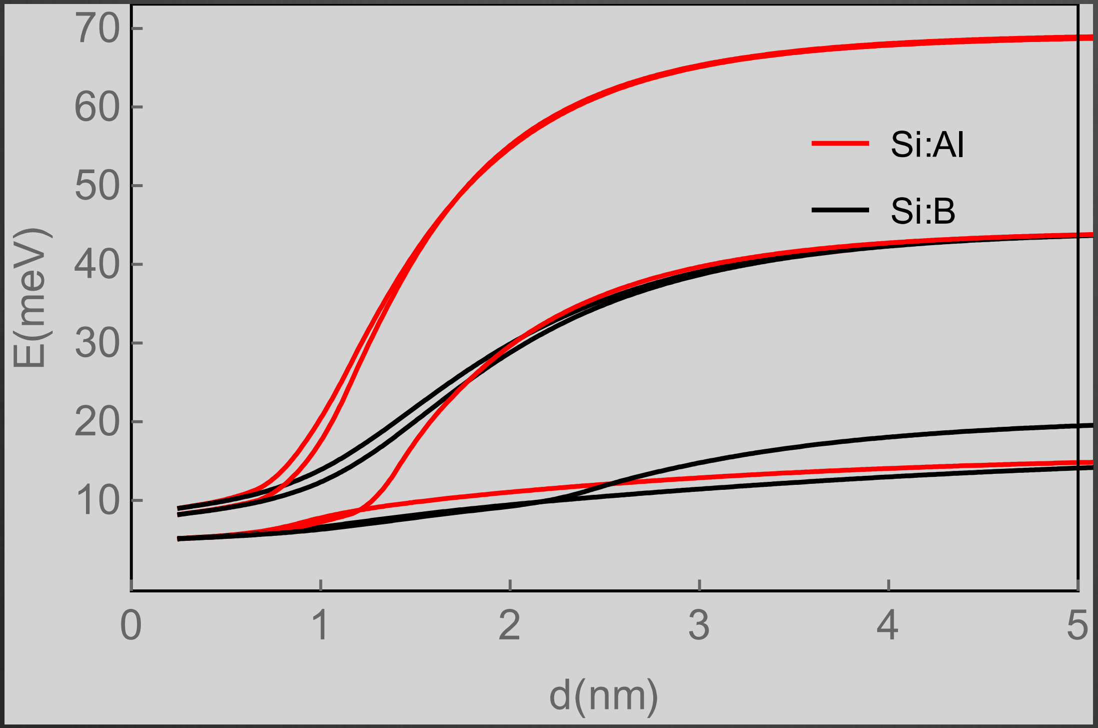
EFFECT OF IMAGE CHARGES



Enhanced binding,
reduced compression

For Si/SiO_2 interface Q'=-0.5
For Si/vacuum interface Q'=-0.84 → larger enhancement

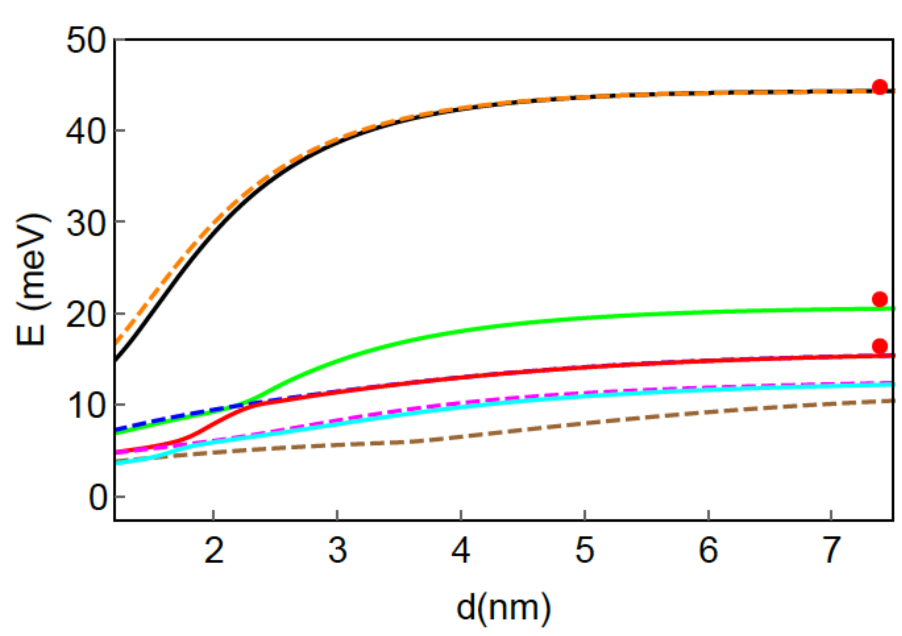
EFFECT OF CENTRAL CELL

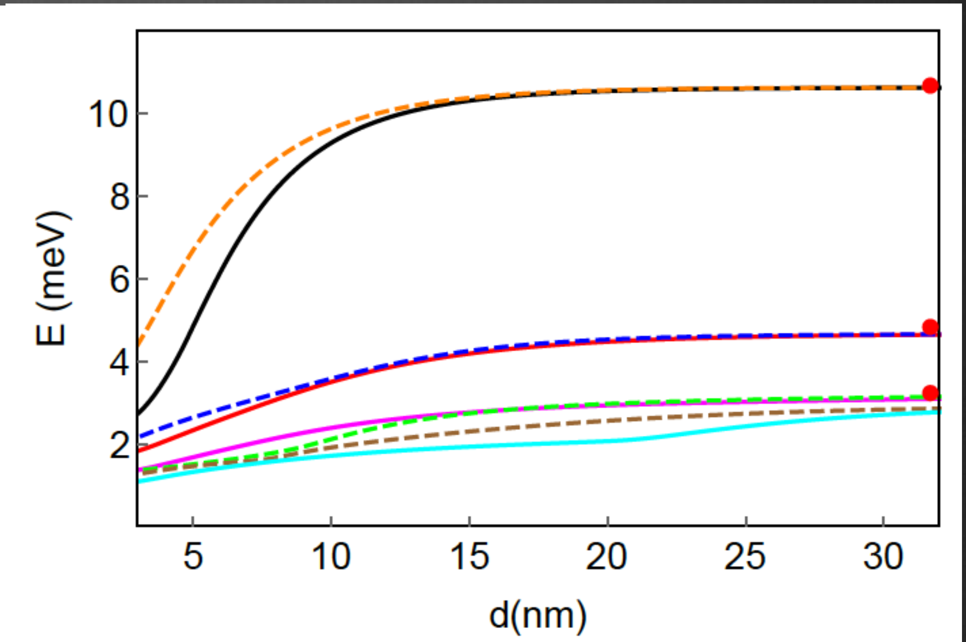


$$V_{cc} = \frac{2(\epsilon_s - 1)e^{-r/r_{cc}}}{r}$$

The interface deforms the hole wf away from the Coulomb center.
So, near the interface the CC effects are lost.

GERMANIUM





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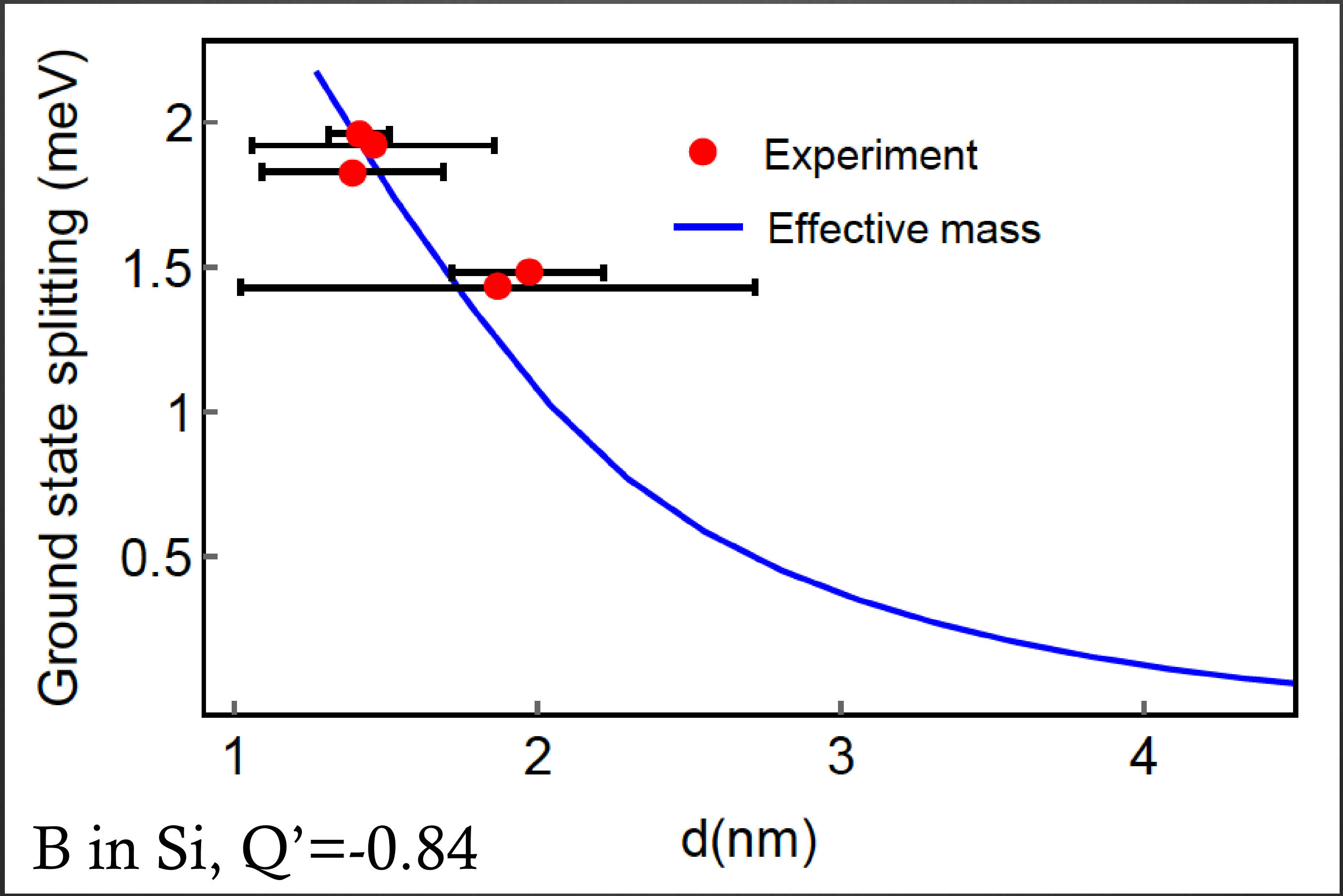
Si:B GROUND STATE SPLITTING



Experimental points from: Mol et al APL 106, 203110 (2015).

CONCLUSIONS

- Quantum confinement leads to a reduction of the binding energies close to the interface and a compression of the energy spectrum.
- Dielectric mismatch with the insulator enhances the binding energy.
- The symmetry reduction at the interface leads to the ground state splitting.
- Similar results are obtained for Ge.
- The reduction of the symmetry by the interface can be used to enhance the dipolar coupling of the acceptors (Culcer et al Nanotechnology, 27, 24 (2016). and Rogge et al. PRL 116, 246801)