Heterointerface effects on the charging energy of shallow D^- ground state in silicon: the role of dielectric mismatch.

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Ref: M.J. Calderón, J. Verduijn, G.P. Lansbergen,
G.C. Tettamanzi, S. Rogge, B. Koiller,
Phys. Rev. B 82, 075317 (2010)

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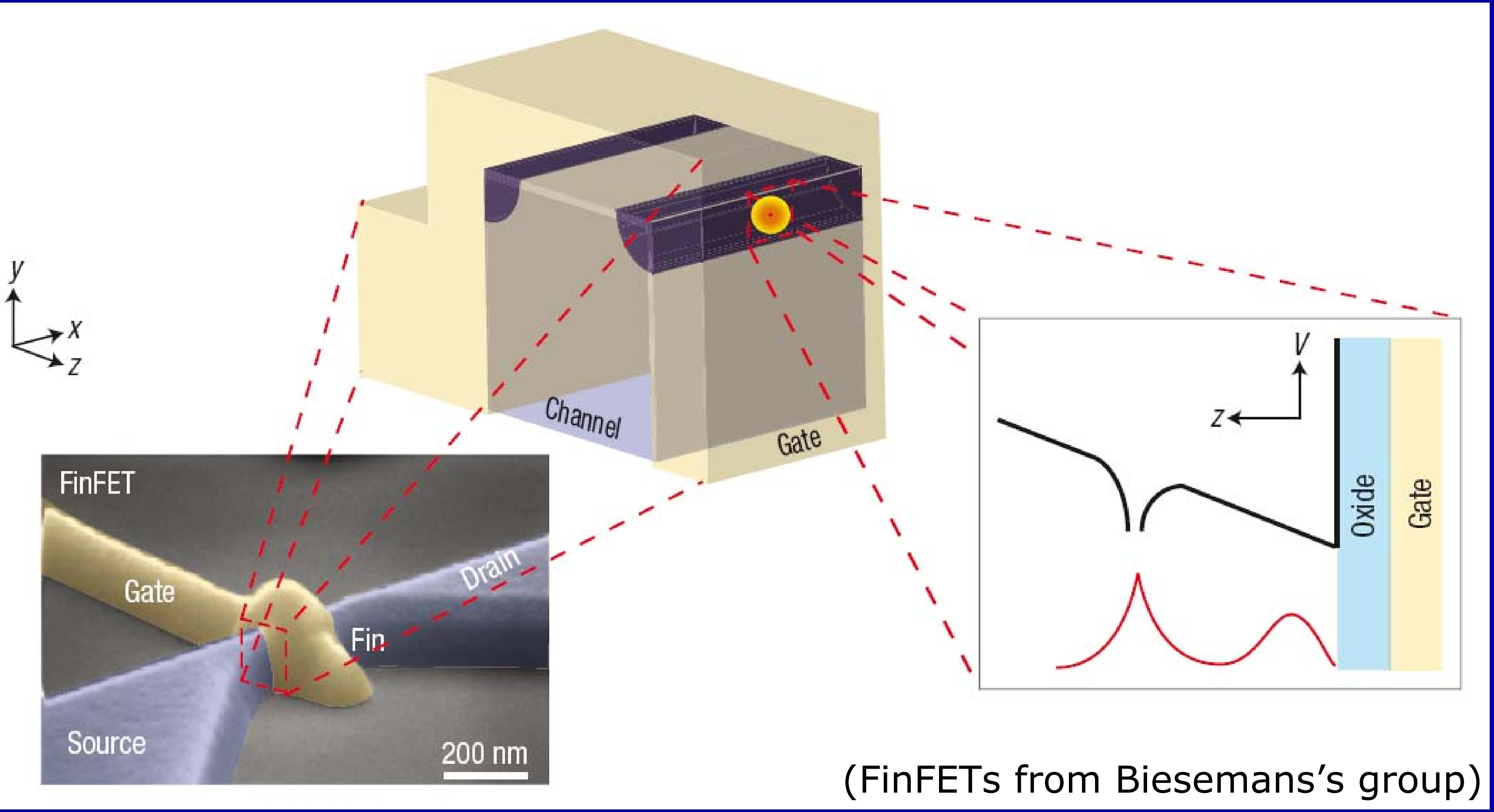
MOTIVATION
FinFET: single donor detection device

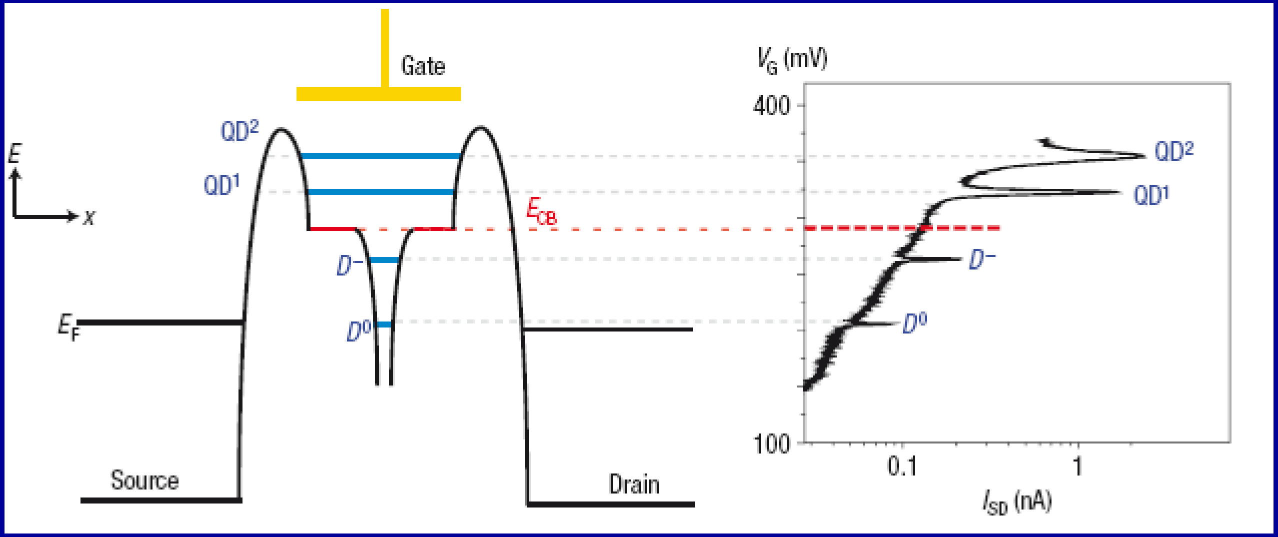


Arsenic donors may diffuse from source or drain to the channel

Sellier et al, PRL (2006)
Lansbergen et al, Nat. Phys. 4, 656 (2008)

MOTIVATION

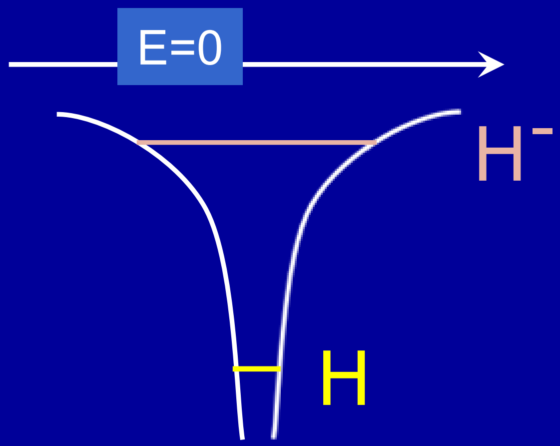
FinFET: transport spectroscopy



✓ Two resonances, corresponding to the 2 possible donor bound states (D^0 and D^-) are observed below the conduction band.

Lansbergen et al, Nat. Phys. 4, 656 (2008)

Hydrogen bound charge states



Negatively charged ion: H^- ($H^+ + 2e^-$)

$E_{H^-} < 0$

Neutral atom ($H^+ + 1e^-$), $E_H < 0$

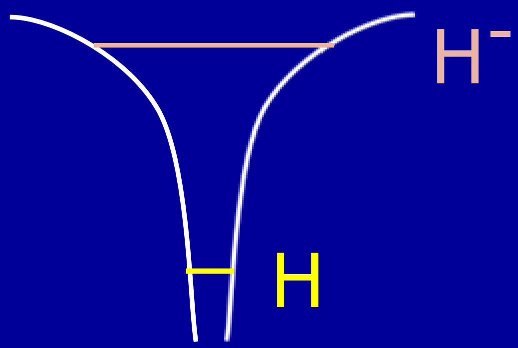
$$U_{coul} = -\frac{e^2}{r}$$

Binding energy for H^-

$$E_B^{H^-} = E_H - E_{H^-} \ (> 0)$$

H. Bethe and S. Salpeter, "Quantum mechanics of one and two electron atoms" Dover

Hydrogen bound charge states



Negatively charged ion: H^- ($H^+ + 2e^-$)

Neutral atom ($H^+ + 1e^-$)

Non-interacting e^- energy for H^-

$$E_{H^-} = 2E_H$$

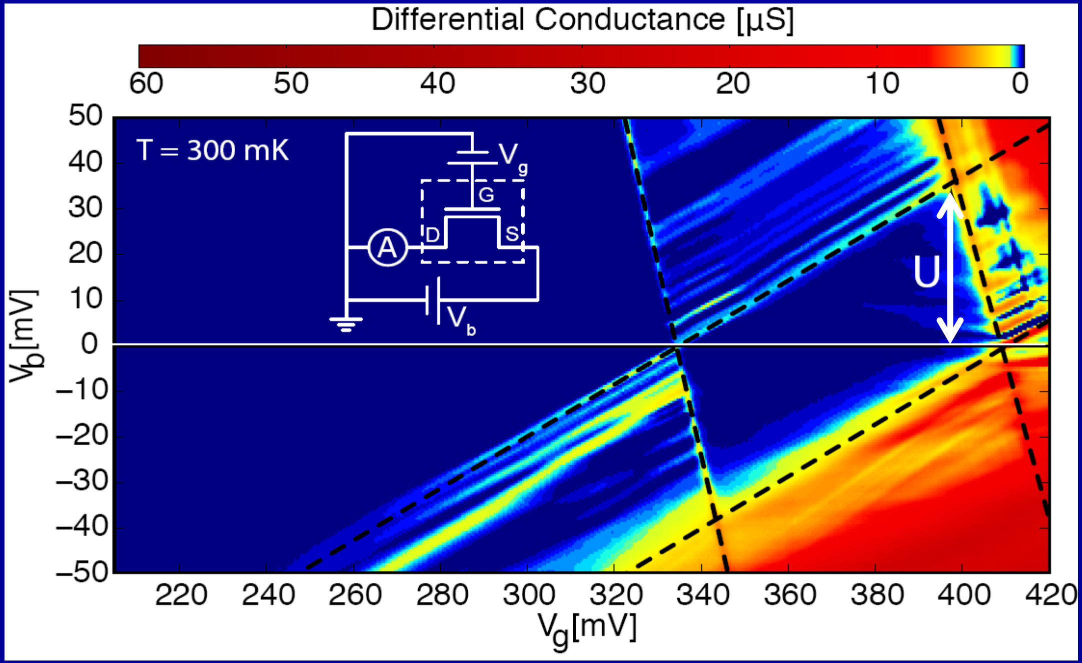
Charging energy:
~ $e^- \leftrightarrow e^-$ repulsion

$$E_{H^-} = 2E_H + U \quad \Rightarrow \quad U = E_{H^-} - 2E_H > 0$$

H. Bethe and S. Salpeter, “Quantum mechanics of one and two electron atoms” Dover

Stability diagram
Fin FET Experiments

Charging energy
U= 36±1 meV



Similar values found in other samples (U~28-36 meV)

However, U_{As} in bulk Si ~52 meV

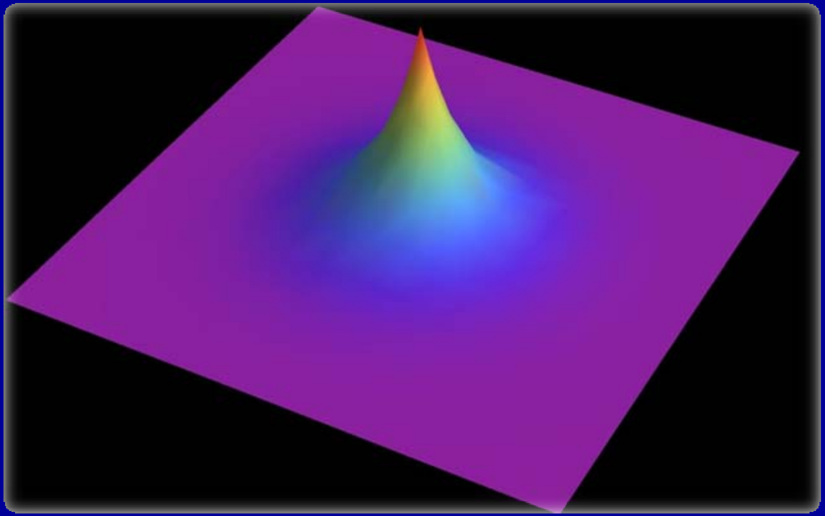
Where does the reduction in U come from?

We investigate the role of the dielectric mismatch at the interface.

Neutral hydrogen atom H^0

Hamiltonian for 1 electron

$$h(r) = -\nabla^2 - \frac{2}{r}$$



Ground state $$\phi_{1s}(r,a) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$ with $a = 1 a_B$ and $E_H = -1 Ry$

Atomic units are adopted here

$$a_B = \frac{\hbar^2}{m_e e^2} = 0.5\,\mathring{A}$$

$$Ry = \frac{m_e e^4}{2\hbar^2} = 13.6\,\mathrm{eV}$$

Negative hydrogen ion H^-

Proton + e- + e-

Hamiltonian for 2 electrons

$$H_{bulk} = h(r_1) + h(r_2) + \frac{2}{|\vec{r}_1 - \vec{r}_2|}$$

Variational trial ground state function (spin singlet)

$$|1s,1s,s\rangle = \left[\phi_{1s}(r_1,a)\,\phi_{1s}(r_2,b) + \phi_{1s}(r_1,b)\,\phi_{1s}(r_2,a)\right]\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

Results

$$E^{H^-} = -1.027Ry \quad \Rightarrow E_B^{H^-} = 0.027Ry, \quad U = 0.973Ry$$

$$a = 0.963\,a_B \quad \text{(effective Bohr radius of inner orbital)}$$

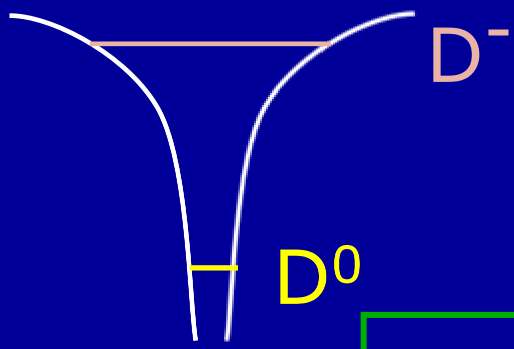
$$b = 3.534\,a_B \quad \text{(effective Bohr radius of outer orbital)}$$

} Variational

Shallow donors in bulk Si within hydrogenic analogy

$$Ry \rightarrow Ry^* = \frac{m^* e^4}{2\varepsilon_{\text{Si}}^2 \hbar^2} = 31.2\text{ meV}$$

$$a_B \rightarrow a^* = \frac{\hbar^2 \varepsilon_{\text{Si}}}{m^* e^2} = 2.14\text{ nm}$$



$$U_{Coul} = -\frac{2}{\varepsilon_{\text{Si}} r}$$

$$E^{D^0} = -1Ry^*$$

$$E^{D^-} = -1.027Ry^*$$

$E_B^{D^-} = 0.027Ry^* \rightarrow$ binding energy

$U = 0.973Ry^* \rightarrow$ charging energy

Theoretical bulk values

	D (Ry*)	D (meV)
$E_B^{D^0}$	1	31.2
$E_B^{D^-}$	0.027	0.84
U	0.973	30.36

Experimental bulk values

	P	As
$E_B^{D^0}$ (meV)	45	54
$E_B^{D^-}$ (meV)	1.7	2.05
U (meV)	43.3	51.95

Approximations

✓ Isotropic mass: $m^* \sim 0.3\ m_e$

✓ Single valley

✓ Flat band (no electric field)

✓ Simple variational wave-function

Not included:

Mass anisotropy
($m_\perp = 0.191\ m_e$, $m_{||} = 0.916\ m_e$)

Multivalley conduction band structure

} enhancement of $E_B^{D^0}$ and $E_B^{D^-}$

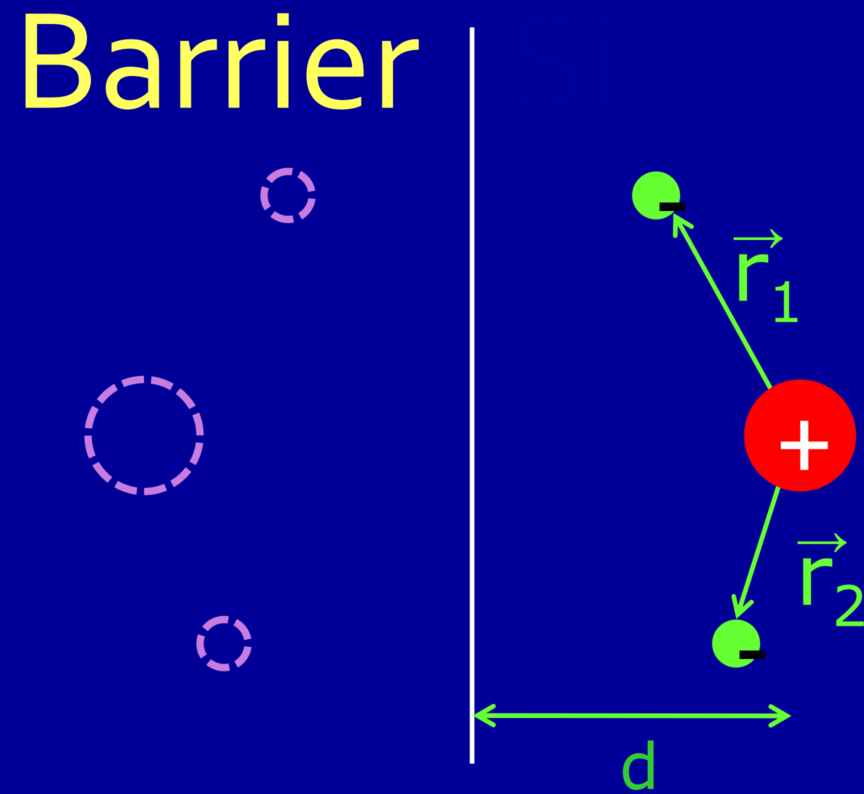
Inoue et al PRB 77, 125213 (2008)
Larsen PRB 23, 5521 (1981)

A more complex variational wave-function (Chandrasekar-type) for D^- increases its binding energy.

Hao et al, arXiv:1005.2315

Boundary problem

Image charges



Boundary problem

Image charges

$$H_{\text{images}}(r_1,r_2) = -\frac{Q}{2(z_1+d)} - \frac{Q}{2(z_2+d)}$$

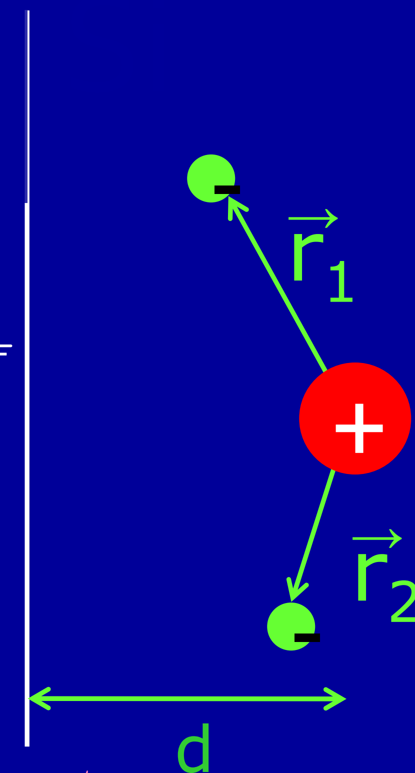
Interaction of each electron with its own image

Interaction of each electron with the donor's image

$$+\frac{2Q}{\sqrt{x_1^2+y_1^2+(z_1+2d)^2}} + \frac{2Q}{\sqrt{x_2^2+y_2^2+(z_2+2d)^2}}$$

Interaction between each electron and the other electron's image

$$-\frac{4Q}{\sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(2d+z_1+z_2)^2}}$$



Dielectric mismatch parameter

$$Q=\frac{\varepsilon_{\text{barrier}}-\varepsilon_{\text{Si}}}{\varepsilon_{\text{barrier}}+\varepsilon_{\text{Si}}}$$

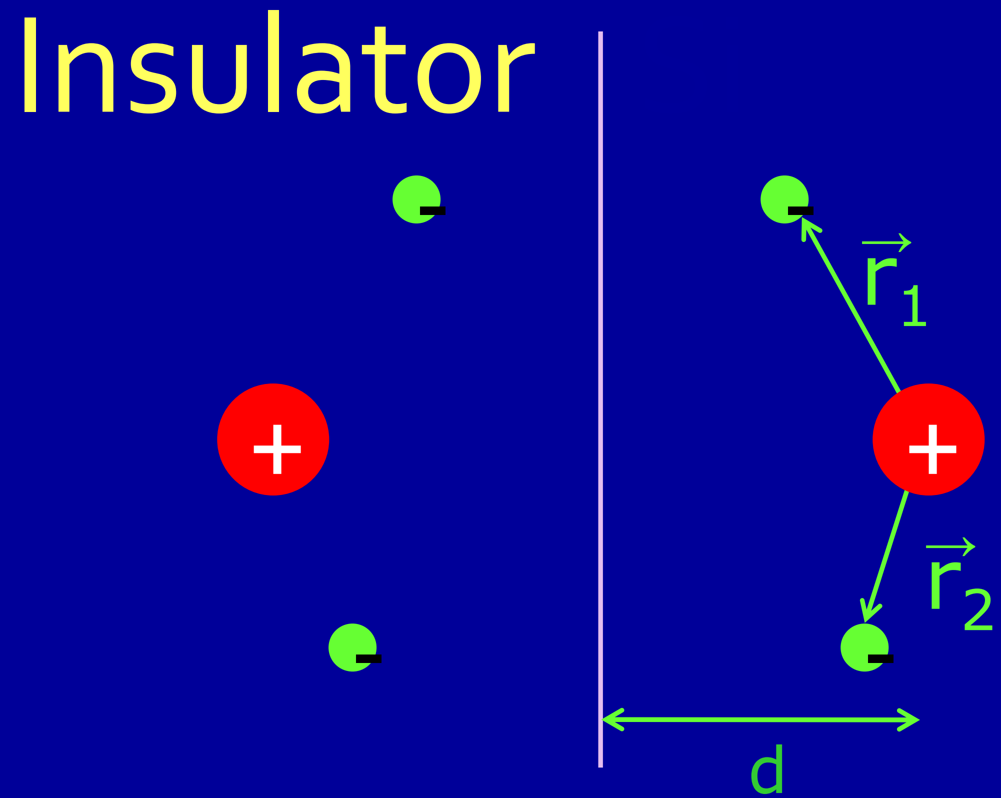
Boundary problem

Image charges

$$Q = \frac{\varepsilon_{barrier} - \varepsilon_{Si}}{\varepsilon_{barrier} + \varepsilon_{Si}}$$

$$\text{Ins. barrier} \Rightarrow Q < 0$$

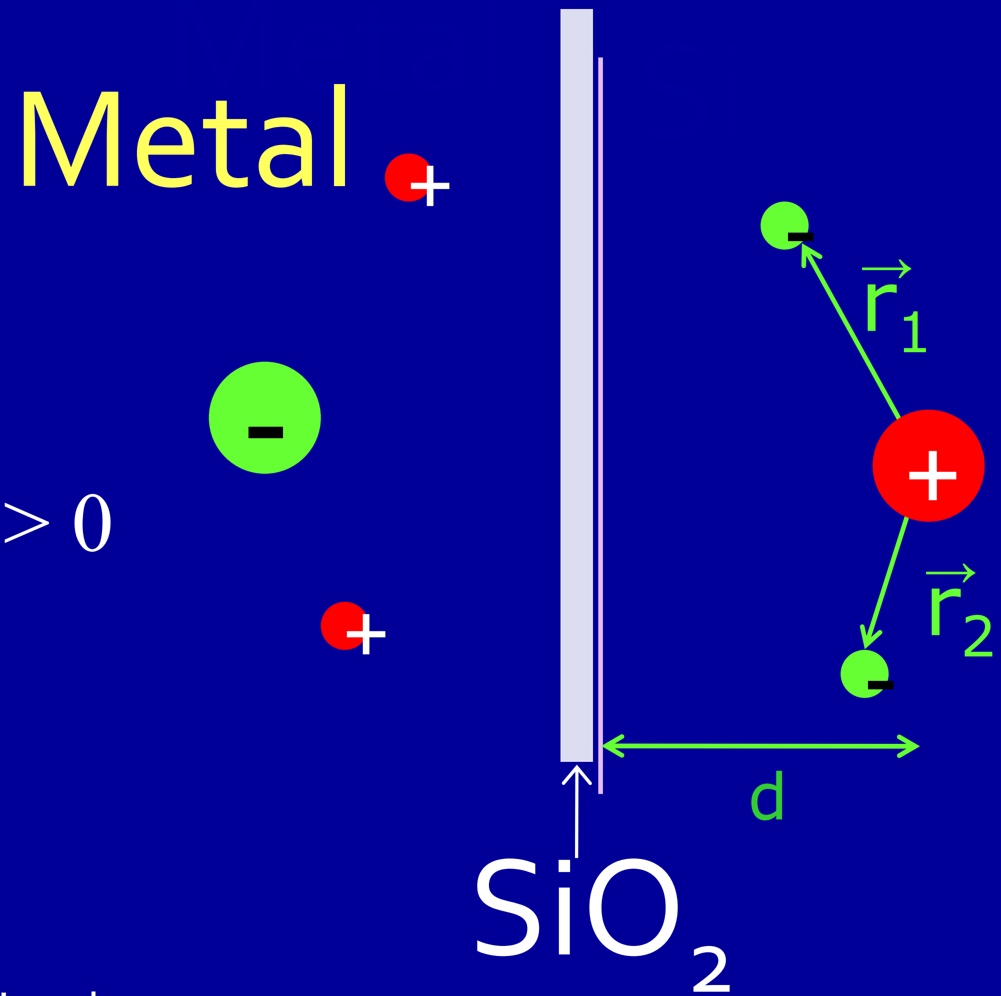
Attractive donor image;
repulsive electron images



Note: A rigorous calculation would involve an infinite set of image charges
Hao et al, PRB 80, 035329 (2009).

Boundary problem
Image charges

$$Q = \frac{\varepsilon_{barrier} - \varepsilon_{Si}}{\varepsilon_{barrier} + \varepsilon_{Si}}$$



$$\text{Thin ins.} + \text{metal} \Rightarrow Q > 0$$

Repulsive donor image;
attractive electron images

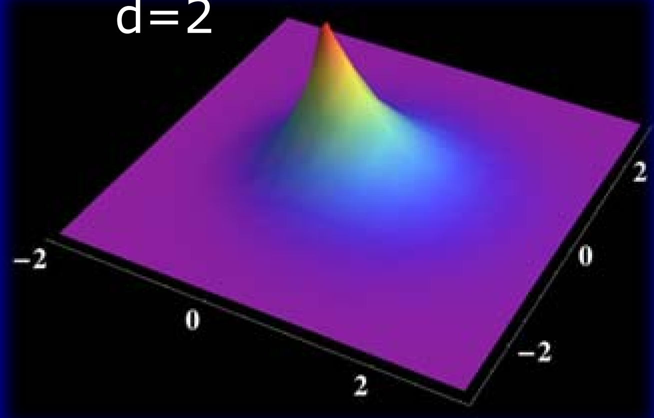
Note: A rigorous calculation would involve an infinite set of image charges
Hao et al, PRB 80, 035329 (2009).

Boundary condition: Ψ(z=-d)=0

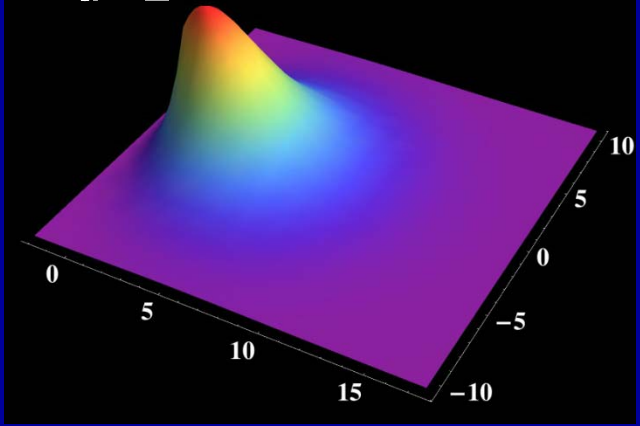
imprenetrable barrier at z=-d

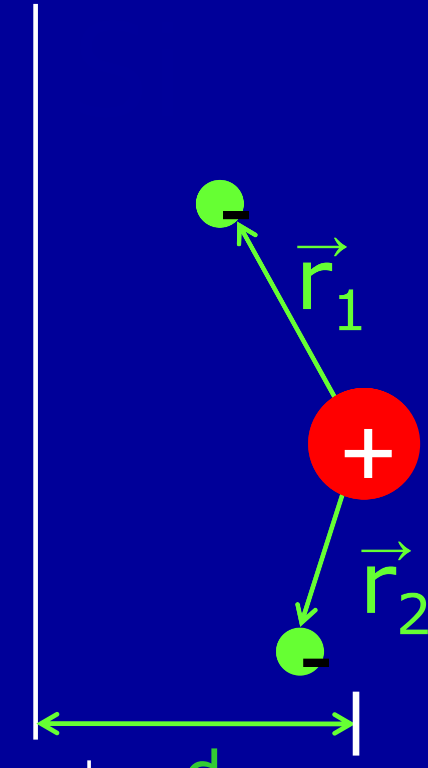
a, b and d In units of a* = 2.14 nm

a=1 (inner orbital)
d=2



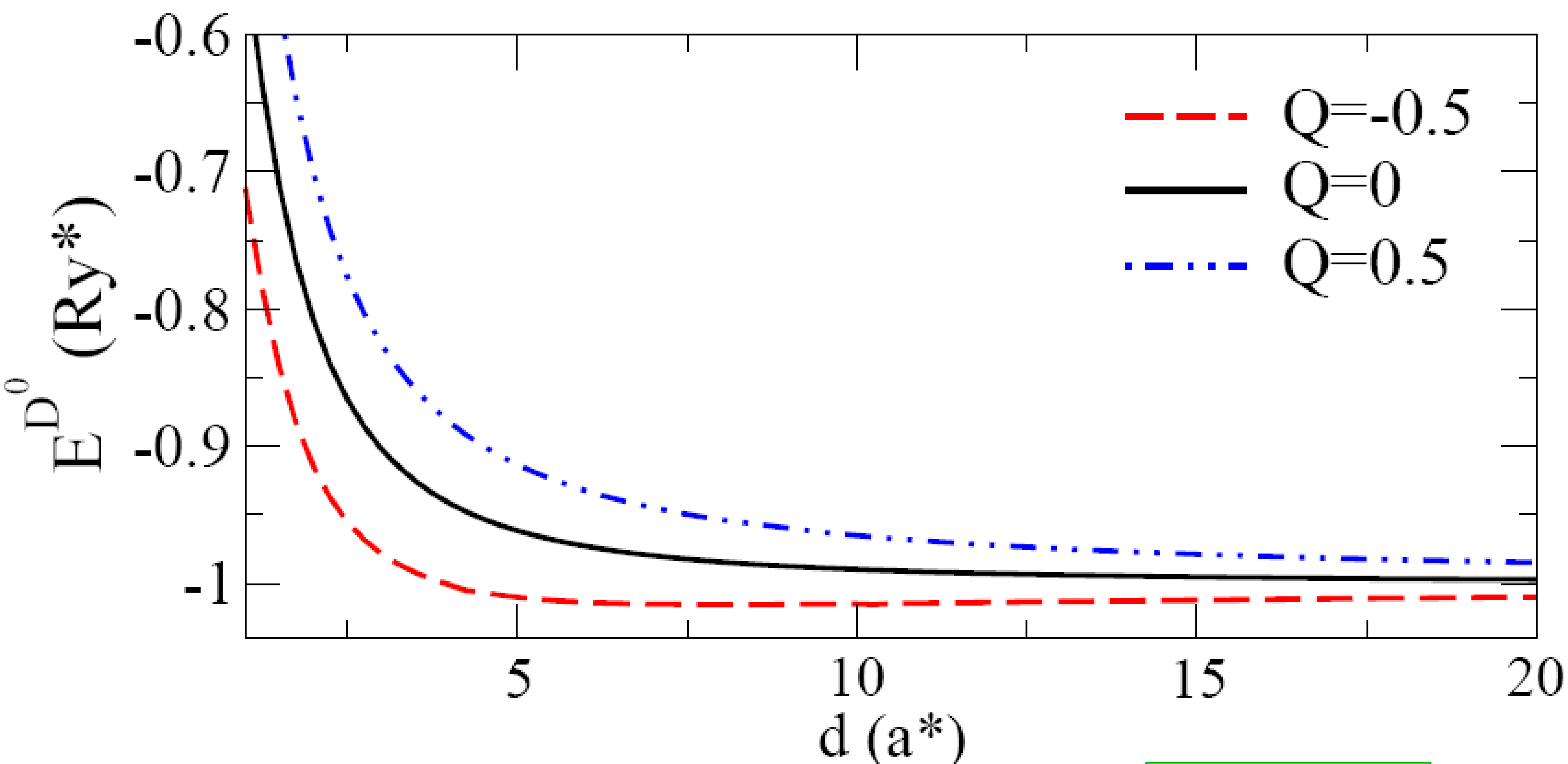
b=3.53 (outer orbital)
d=2





$$\phi_{1s}(r,a) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a} \left(z + d \right)$$

Results for a neutral donor (D^0)



$Ry^* = 31.2$ meV

$a^* = 2.14$ nm

Q=-0.5 → thick SiO_2 barrier

Q=0 → no images

Q=0.5 → *effective* Q for thin SiO_2 + metal layer

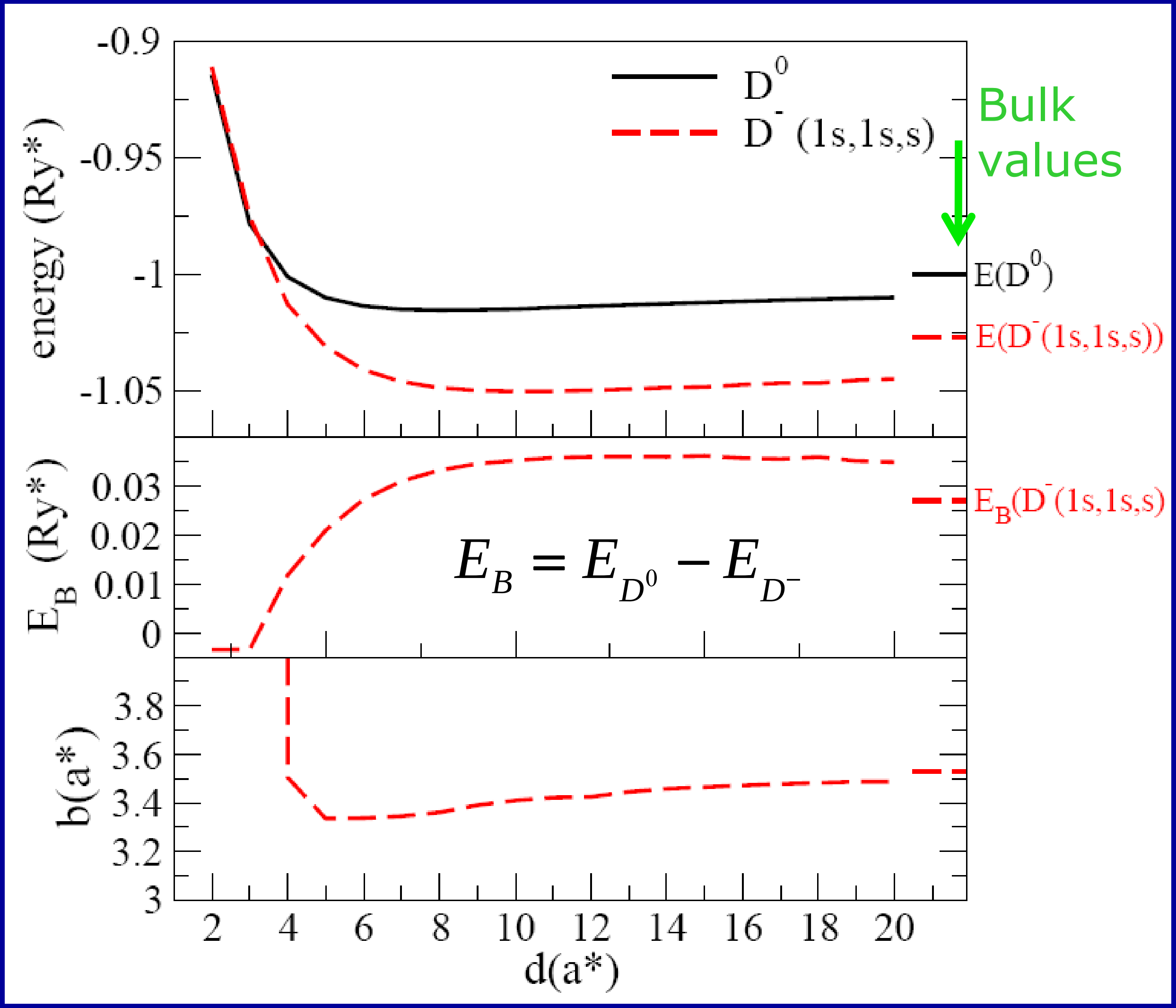
Results for D^-

Q=-0.5 → thick SiO_2 barrier

$Ry^* = 31.2$ meV

$a^* = 2.14$ nm

- Bulk values are approached as *d* increases.
- D^- is not bound for *d*<4 a*. For small *d* the outer orbital radius *b* diverges.
- Binding energy is enhanced with respect to bulk for *d* ≥ 3 a*.
- Radius of inner orbital *a* similar to D^0 at all *d*.



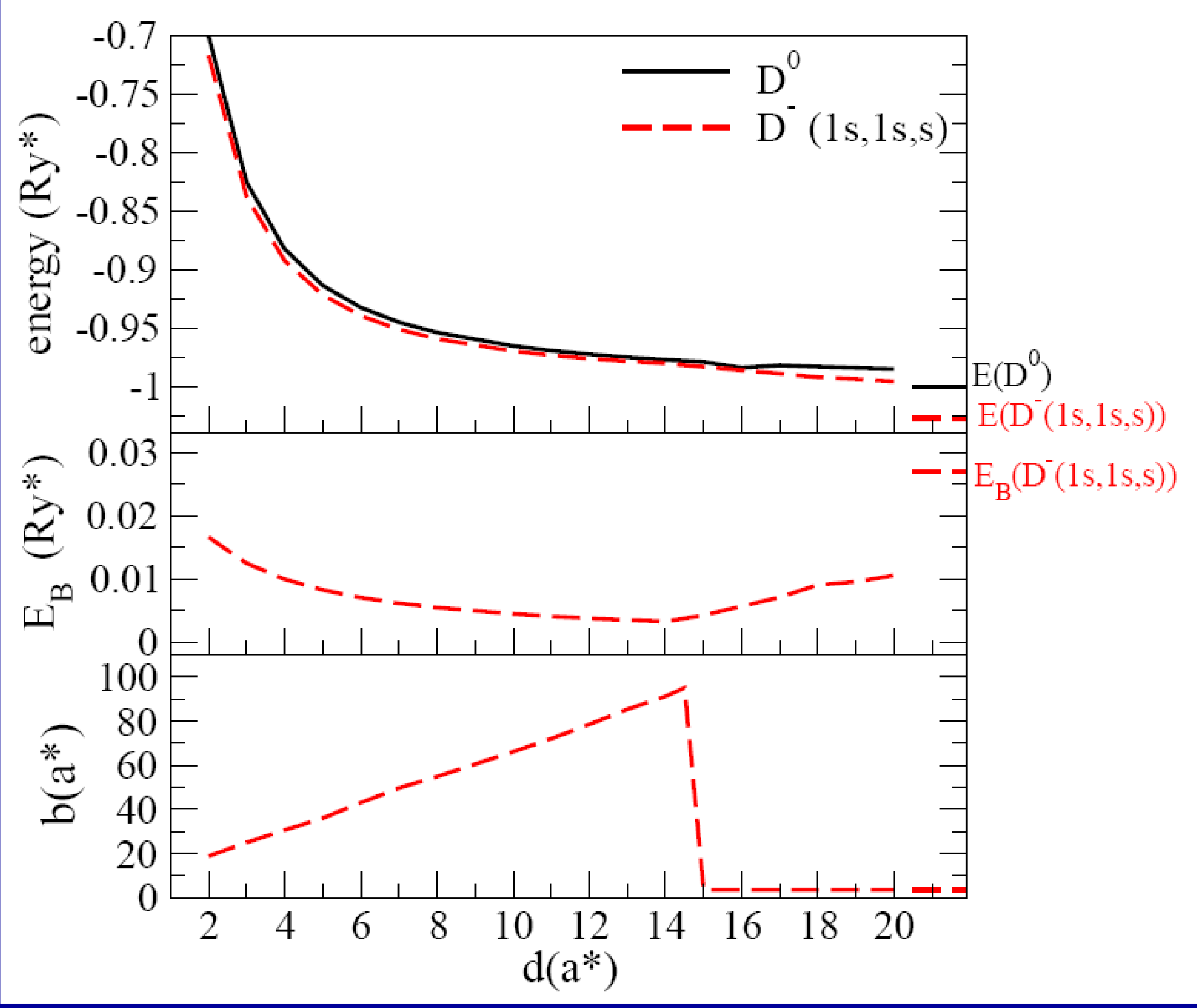
Results for D^-

Q=+0.5 → ~ thin SiO_2 barrier + metal layer

$Ry^* = 31.2$ meV

$a^* = 2.14$ nm

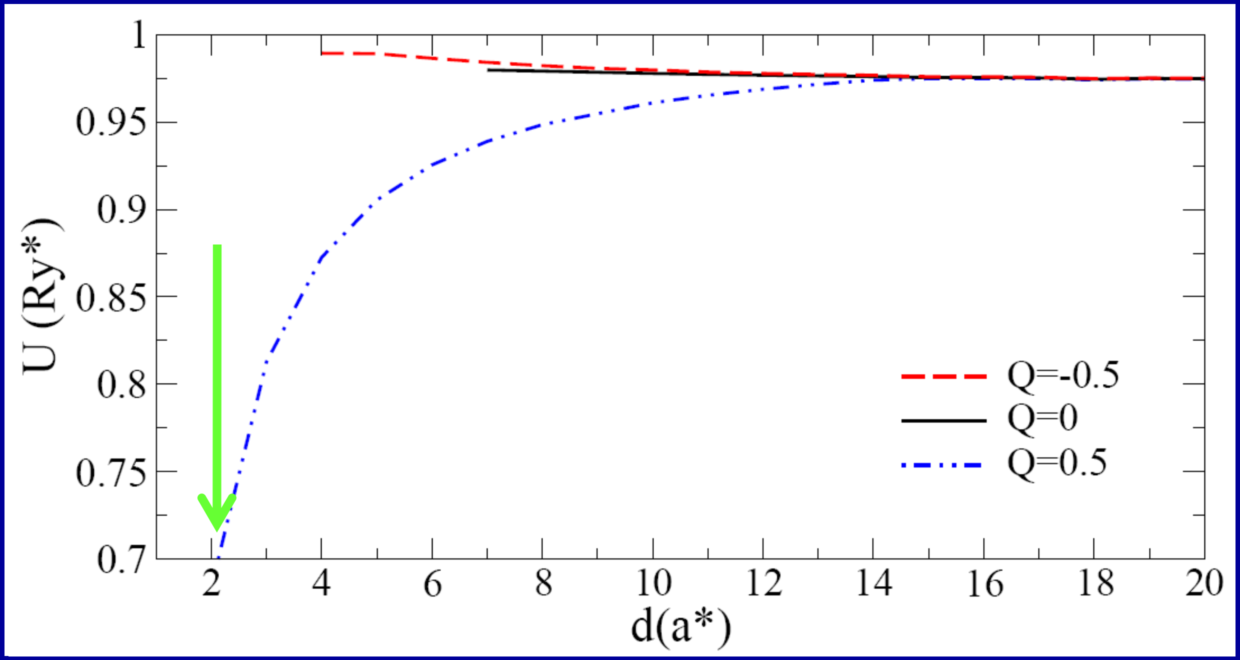
- Bulk values are approached as *d* increases.
- D^- is bound at all *d* (*b* is always finite).
- Binding energies are reduced with respect to bulk.



The combined effect of the insulator plus the metallic gate screening may be responsible for the observed reduction of U.

Charging energy for D^-

Reminder: U_{bulk}=52 meV
U_{FinFET}=28-36 meV → Ratio= 0.54-0.70



Q=-0.5 → thick SiO_2 barrier

Q=0 → no images

Q=0.5 → effective for thin SiO_2 + metal layer

$$U = E_{D^-} - 2E_{D^0}$$

Conclusions

- ✓ The energy spectrum of isolated donors in Si nanostructures differs from the bulk values. In particular, the charging energy of D^- charged donors is found to be smaller.

- ✓ We show that the proximity of metallic gates, separated from Si by a barrier material, modifies the binding energy of donors and, as a consequence, the charging energy for small distances between donor and interface is reduced.

- ✓ As a first approach to the problem, the combined effect of a barrier and metallic gates on nearby donor levels in Si is conveniently incorporated in a single dielectric mismatch parameter *Q*.

Collaborators

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Relate work (D^0)

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