Towards a disorder model for the Si/SiO_2 interface

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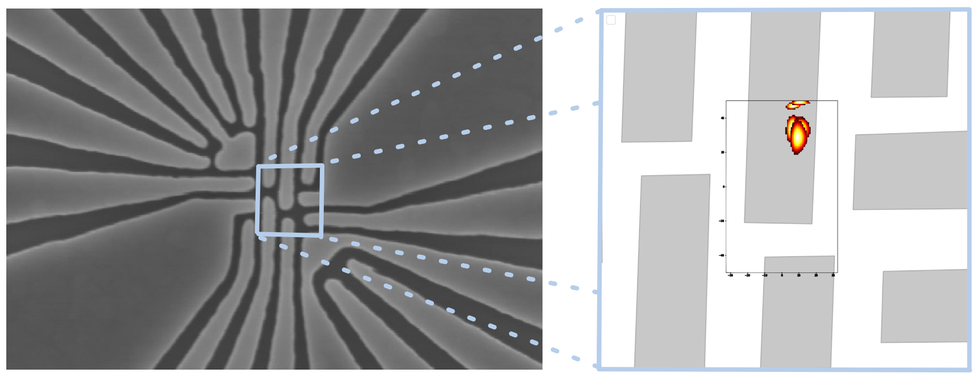
Motivation

Disorder at the Si/SiO2 interface impacts measurements at all stages of qubit development

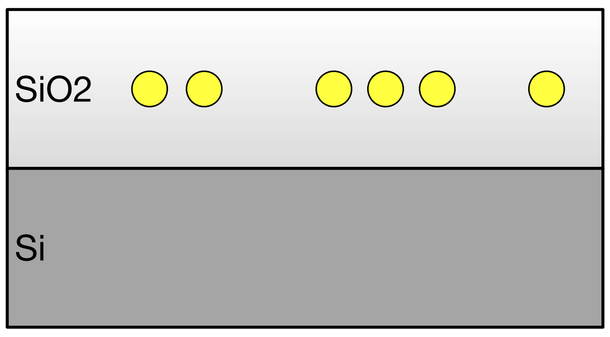
- Inhibits peak mobility in material characterization [1]
- Impacts valley splitting in few-electron dot tuneup [2]
- Lifting of spin blockade in DQDs [3]
- Limits T2* times in working DQD qubits [4]
- Confounds stability diagrams when hunting for donors [5]



Can we develop a physics-based model that is mutually consistent with the wide array of available measurements?

- Focus on electrostatic disorder (i.e., charges in oxide)
- Neglect interface roughness and strain (future work)
- Start with measurements that can be taken at 1K

Model



Parameters

Areal density (10^9-10^{12} cm^{-2})

Distance from interface (1-10 nm)

Effective mass theory

Used to constrain surface roughness from single electron valley splitting measurements [2]

$$\left[-\frac{\nabla_\rho^2}{2m_\perp} - \frac{\nabla_z^2}{2m_\parallel} + U_{disorder}(\mathbf{r})\right] F(\mathbf{r}) = EF(\mathbf{r})$$

$$U_{disorder}(\mathbf{r}) = \sum_{n=1}^{N_c} \frac{Q_{eff}}{4\pi\varepsilon_{Si}|\mathbf{r}-\mathbf{R}_n|} + U_{offset}\theta(z)$$

$$Q_{eff} = \left(\frac{2\varepsilon_{Si}}{\varepsilon_{Si}+\varepsilon_{SiO_2}}\right) e \approx 1.5e$$

Ewald summation is used to evaluate the disorder potential within a doubly-periodic supercell (O(100 nm))

Why a planar distribution of defect charges?

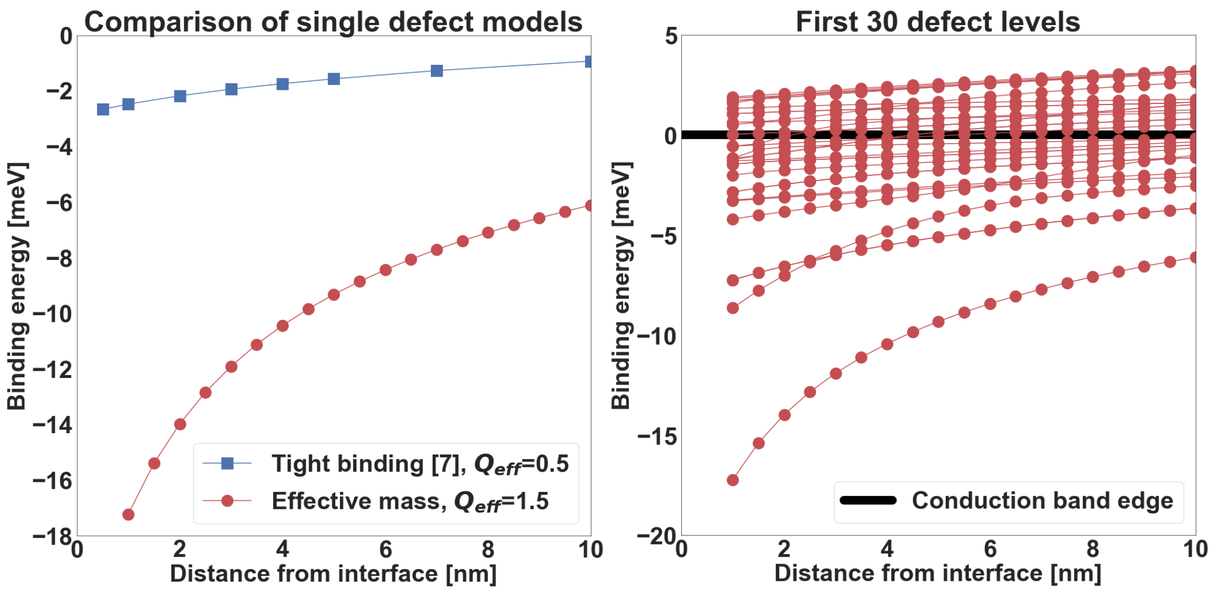
- Assumed in commonly used mobility models [6]
- Insights extensible to SiGe stack
- Generalization to non-planar is trivial

Calculations use Laconic software package

- Discontinuous Galerkin based PDE solver
- Accurately captures sharp solution features close to (nearly) singular trap potentials using a mesh with a fixed resolution

Results

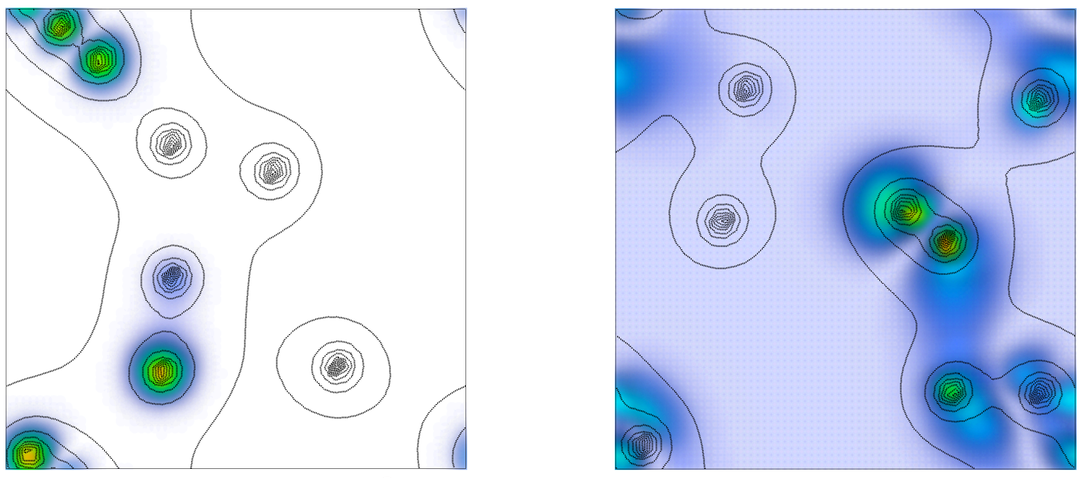
Single defect properties



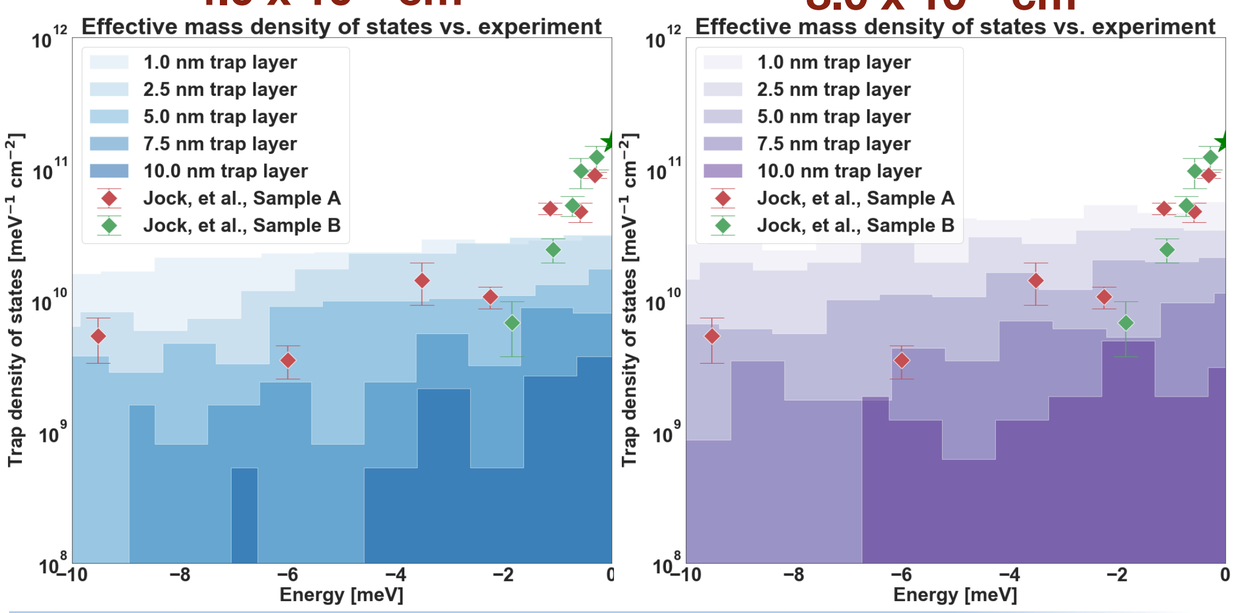
Compare to ESR measurement of trap DOS [7]

Densities: 2.0, 4.0, 8.0 x 10^{10} cm^{-2}
Distances: 1.0, 2.5, 5.0, 10.0 nm
Disorder averaging is over ~1 square micron

Charge density of localized states below (left) and above (right) the conduction band edge



4.0 x 10^{10} cm^{-2} **8.0 x 10^{10} cm^{-2}**



Outlook

- Use effective mass to extract a capacitance model
- Determine whether charge sensing can help distinguish disorder dots and donors
- Correlate this same model against other measurements (e.g., mobility vs density)
- Ultimately, inform a model for charge noise

References

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