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Optimizing the properties of defects at Si surfaces using quantum confinement and strain[1] PETER SCHERPELZ, Institute for Molecular Engineering, University of Chicago, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago and Materials Science Division, Argonne National Laboratory — By manipulating hydrogen-passivated silicon surfaces with an STM tip, dangling bonds (DBs) can be created, which behave as quantum dots with potential applications for quantum information technology. Here we use density functional and many-body perturbation theory calculations to study a single DB on Si(100), and demonstrate how the properties of DB states can be altered in order to design the behavior of DB quantum dots. We show that while in thick Si films the singly-occupied DB state is resonant with the bulk valence band, in quantum-confined thin films the state is an isolated impurity state in the band gap. We also find that strain can further isolate DBs in the gap of the material, depending on the sample geometry and morphology. Finally, we calculate charge transition levels and show how these also depend on the sample structural properties. These findings suggest new methods for tuning the properties of defects used in quantum information, and also inform on the parameters required to perform converged simulations of silicon surfaces.

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Peter Scherpelz
Institute for Molecular Engineering, University of Chicago

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