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Isolation of dangling bond states on Si(100) surfaces for quantum information applications PETER SCHERPELZ, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — Hydrogen resist lithography allows dangling bonds to be created and manipulated on Si(100) surfaces, both for use as a controlled quantum system, and as a step in the deterministic placement of dopants at the single-atom level. However, previous experiments and computations [1] have shown conflicting results on the location of dangling bond energy levels, which can impact their utility as qubits. Here we use large-scale density functional theory and many-body perturbation theory (GW) calculations to show that in clean, H-passivated Si(100)-(2x1) surfaces a singly-occupied dangling bond does not give rise to an electronic state isolated from the valence bands. However, very thin (1-3 nm) samples terminated by a (100) surface should provide isolated singly-occupied and doubly-occupied dangling bond states. We also explore the effect of strain, and consider novel uses of boron dopants. [1] See e.g. Bellec et al. Phys. Rev. B (2013), Ye et al. Surf. Sci. (2013), Schofield et al. Nat. Commun. (2013), Wieferink et al. Phys. Rev. B (2010).

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