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Giant valley splitting in Si/oxide: discriminating Fang-Howard or Tamm-Shockley interface states AMINTOR DUSKO, BELITA KOILLER, Instituto de Física - UFRJ, ANDRÉ SARAIVA, UFRJ / University of Wisconsin - Madison — The conduction band of silicon presents six inequivalent degenerate minima, or valleys. The presence of an abrupt interface lifts this degeneracy by 0.1-1 meV, an energy scale that may directly affect spin qubits. Experiments reporting splittings over 20 meV [1] cannot be explained by this mechanism. Extended Si/oxide interface (Tamm-Shockley) states may account for this enhancement [2]. We present a renormalization solution for the 1D tight-binding (TB) model of this structure [2], so that the full range of TB parameters is readily accessible [3]. The renormalization language naturally reveals the role played by the chemical bond of atoms across the interface. Our approach eliminates the need for a supercell calculation [2], proving the formation of intrinsic interface states regardless of electric field. Moreover, the decimation rate of convergence provides quantitative estimates for the localization lengths of these states. We compare these interface states to the usual field-bound Fang-Howard states, suggesting capacitance measurements to differentiate them [3].

[1] K. Takashina, et al, PRL 96, 236801 (2006)

[2] A. L. Saraiva et al, PRB 82, 245314 (2010)

[3] A. Dusko et al., Phys. Rev. B 89, 205307 (2014)

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