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Localization of Si/SiO_2 Interface States: Properties and Physical Implications[1] BELITA KOILLER, AMINTOR DUSKO, ANDRE SARAIVA, Physics Institute, Universidade Federal do Rio de Janeiro — Interface states (IS) form spontaneously at some semiconductor-barrier interfaces and they may improve or hinder electronic control and coherence for semiconductor-based qubits. Intrinsic Si/SiO_2 IS and its hybridization to the Si bulk states were recently investigated within tight binding (TB) models [1]. From the simplest model (1D), new insights emerge regarding the IS's energy and hybridization with the band states. In this work the 1D TB Hamiltonian is further explored, here within a Green's function formalism. The problem is solved exactly via a decimation technique based on renormalization group ideas [2]. The IS thus obtained are strictly related to the junction of two semi-infinite chains modeling the Si material and the SiO_2 barrier, excluding possible contributions from parameters (e.g. chain length) previously invoked [1]. We obtain the energy of IS as well as the exponential longer (shorter) localization lengths into the Si (barrier) material. The IS may be probed experimentally by an external electric field, which modulates the capacitance of the system, or by the spacing between the two lowest levels, related to the valley splitting [1].

[1] Saraiva et al, Phys. Rev. B 82, 245314 (2010).
[2] da Siva and Koiller, Solid State Commun. 40, 215 (1981)

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