

Abstract Submitted
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Impact of the valley degree of freedom on the control of donor electrons near a Si/SiO₂ interface¹ ANDRE SARAIVA, IF-UFRJ, ALEJANDRA BAENA, MARIA CALDERÓN, ICMM - CSIC, BELITA KOILLER, IF-UFRJ — We analyze the valley composition of one electron bound to a shallow donor close to a Si/barrier interface as a function of an applied electric field within a multivalley effective mass model. Switching from low to high fields, the electron ground state is drawn from the donor site into the interface, leaving the donor partially ionized. Valley splitting at the interface occurs due to the valley-orbit coupling, $V_{vo}^I = |V_{vo}^I|e^{i\theta}$. At intermediate electric fields, close to a characteristic shuttling field, the electron states may constitute hybridized states with valley compositions different from the donor and the interface ground states. The full spectrum shows crossings and anticrossings as the field varies. The degree of level repulsion depends on the relative valley compositions, which vary with $|V_{vo}^I|$, θ and the interface-donor distance. We focus on the valley configurations of the states involved in the donor-interface tunneling process, given by the anticrossing of the three lowest levels. A sequence of two anticrossings takes place and the complex phase theta affects the symmetries of the eigenstates and level anticrossing gaps. Implications of our results on the practical manipulation of donor electrons in Si nanostructures are discussed.

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