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Atomistic analysis of valley-orbit hybrid states and inter-dot tunnel rates in a Si double quantum dot RIFAT FERDOUS, RAJIB RAHMAN, GERHARD KLIMECK, Purdue Univ — Silicon quantum dots are promising candidates for solid-state quantum computing due to the long spin coherence times in silicon, arising from small spin-orbit interaction and a nearly spin free host lattice. However, the conduction band valley degeneracy adds an additional degree of freedom to the electronic structure, complicating the encoding and operation of qubits. Although the valley and the orbital indices can be uniquely identified in an ideal silicon quantum dot, atomic-scale disorder mixes valley and orbital states in realistic dots. Such valley-orbit hybridization, strongly influences the inter-dot tunnel rates.Using a full-band atomistic tight-binding method, we analyze the effect of atomic-scale interface disorder in a silicon double quantum dot. Fourier transform of the tight-binding wavefunctions helps to analyze the effect of disorder on valley-orbit hybridization. We also calculate and compare inter-dot inter-valley and intra-valley tunneling, in the presence of realistic disorder, such as interface tilt, surface roughness, alloy disorder, and interface charges. The method provides a useful way to compute electronic states in realistically disordered systems without any posteriori fitting parameters.

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