Abstract Submitted
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Genetic Design of Enhanced Valley Splitting towards a Spin Qubit in Silicon[1] LIJUN ZHANG, JUN-WEI LUO, National Renewable Energy Laboratory, ANDRE SARAIVA, BELITA KOILLER, Universidade Federal do Rio de Janeiro, Brazil, ALEX ZUNGER, University of Colorado — The quantum state of an electron in the Si conduction band holds exceptional promise for quantum computing, owing to its attractive spin coherence properties and adaptability to standard electronics. A paramount challenge is the orbital degeneracy of the lowest conduction band of Si, which is potentially a serious source of decoherence for spin qubits. Hence, isolating a single electron valley state by creating a sufficiently large valley splitting (VS) is a prerequisite for the realization of Si-based spin qubits. Previous explorations of Si quantum wells confined by Si-Ge alloy barriers led thus far to a limited VS of the order of 1 meV or smaller. Here we demonstrate, via an atomically resolved pseudopotential theory, that the monolayer ordering of Si-Ge barriers within reach of modern superlattice growth techniques can be harnessed to enhance the VS by up to one order of magnitude compared to disordered random alloy barriers. A biologically inspired genetic-algorithm search allowed us to identify magic atomic layer sequences of the superlattice barriers that isolate single electron valley state in Si with VS as large as ∼9 meV. These results may provide a roadmap for reliable spin-only quantum computing in Si.

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