Electron Exchange Interaction in Electronically Confined Si Quantum Dots

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Electron exchange interactions in electronically confined Si quantum dots are modeled with an $sp^3d^5s^*$ empirical tight-binding model. Previous work has shown that the exchange energies for electrons confined by P donors in bulk Si display a fast oscillatory behavior with respect to the inter-donor distance [1]. This result implies that P donors need to be positioned with atomic-scale precision in order to implement a Si:P based quantum computer architecture. In contrast to the Si:P architecture, electronically confined Si quantum dots show a simple exponential decay of the exchange energies with the increase of the inter-dot distance. The exponential behavior is attributed to tensile biaxial strain in the Si quantum well, which is epitaxially grown on top of a relaxed Si_xGe_{1-x} layer. The tensile biaxial strain lifts the degeneracy of six valleys in the Si band structure, with the Z valley at lower than the X and Y valleys. The lowest electron wave function originates from the Z valley, and hence Bloch oscillations are present in the z direction only. As a result, when the inter-dot distance changes along the x and y directions, the exchange energy, which is determined by the overlap between the two electron wave functions, does not oscillate.

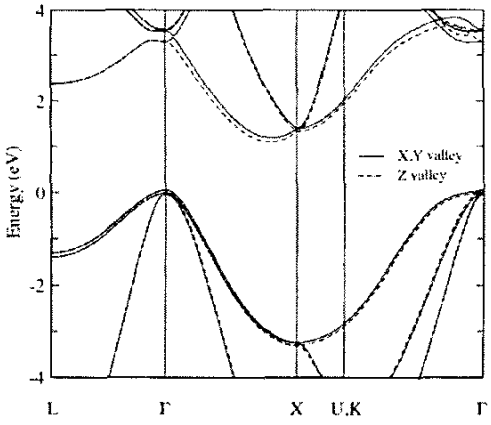

Figure 1. Band structure of biaixially strained Si with tensile strain 0.76% along the x and y directions and compressive strain 0.59% along the z direction. The splitting between the X(Y) valley and the Z valley is about 0.1 eV.

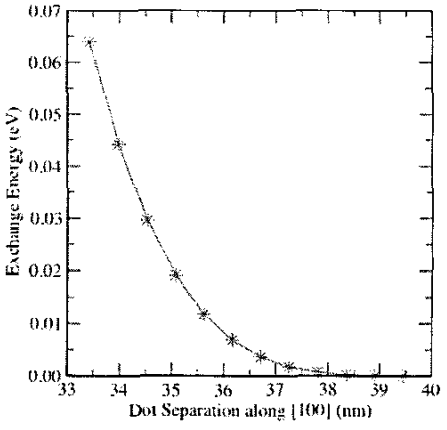

Figure 2. Exchange energies between two electrons confined in Si quantum dots which are electronically confined in a strained Si quantum well, as a function of inter-dot distance along x or y directions. The inter-dot distance is given by the distance between the dot centers. The exchange energy exponentially decays as the inter-dot distance increases.

[1] B. Koiller, X. Hu, and S. Das Sarma, Phys. Rev. Lett. 88, 27903 (2002).

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