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Studying Si/SiGe disordered alloys within effective mass theory[1]
JOHN GAMBLE, Center for Computing Research, Sandia National Laboratories, INÈS MONTAÑO, MALCOLM S. CARROLL, Sandia National Laboratories, RICHARD P. MULLER, Center for Computing Research, Sandia National Laboratories — Si/SiGe is an attractive material system for electrostatically-defined quantum dot qubits due to its high-quality crystalline quantum well interface. Modeling the properties of single-electron quantum dots in this system is complicated by the presence of alloy disorder, which typically requires atomistic techniques in order to treat properly. Here, we use the NEMO-3D empirical tight binding code to calibrate a multi-valley effective mass theory (MVEMT) to properly handle alloy disorder. The resulting MVEMT simulations give good insight into the essential physics of alloy disorder, while being extremely computationally efficient and well-suited to determining statistical properties.

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