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GeVn defects in silicon: a viable route towards room temperature quantum information technology

Abstract:
Defect states in the silicon gap have been exploited in quantum information processing.
While conventional dopants require low-temperature operating conditions, defects characterized by deep energy levels would allow to realize single-atom devices working at room-temperature.
We propose GeVn complexes as good candidates to achieve room temperature single electron operations. These hybrid defects picks up the interesting properties of the vacancy in silicon, which carries deep states in the bandgap, and spatial controllability of the defect by exploiting high precision single ion implantation of Ge, as the two combine in a complex at suitable annealing temperature around 500°C.
By means of ab initio Density Functional Theory (DFT) calculation with screened-exchange hybrid functional, we characterize structural and electronic properties of different GeVn defects.
The calculation of the excitation energies for the addition of electrons to the defect gives deep charge transition levels in the gap, in very good agreement with experimental data.

The high localization of the defect-related states allows a tight binding description of the system.
By mapping the ab initio Hamiltonian in an extended Hubbard one we analyze the conditions for resonant transport in an array of GeV defects.
Moreover we show that due to the very large U/t this system could can be a platform to study the antiferromagnetic correlation at half filling, suggesting a possible exploitation as Hubbard simulator.

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