Ge-V_n complexes in silicon: a viable route toward room temperature quantum information

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The development of on-demand individual deep impurities in silicon is motivated by their employment as a physical substrate for qubits [1], nanoscale transistors [2] and Hubbard-like quantum systems [3]. Single-atom silicon devices based on conventional doping elements such as phosphorous [4], arsenic [5] and boron, as well as other shallow-level dopants can operate only at cryogenic temperature due to their shallow weakly localized ground state impurity levels [6]. Differently, the implantation of Ge dopants in silicon and the subsequent annealing is expected to generate stable Germanium-vacancy defects [7] that are promising candidates to achieve single-atom quantum effects at room temperature.

These hybrid complexes combine indeed the properties of the silicon vacancy, which carries deep states in the bandgap, with the accurate spatial controllability of the defect obtainable through state of the art single-ion implantation of Ge atom.

By means of ab initio Density Functional Theory (DFT) calculation with screened-exchange hybrid functional, that solves the "gap and delocalization problem" of standard DFT, we characterize structural and electronic properties of different Ge-V_n defects. The calculated thermodynamic charge transition levels, corresponding to the excitation energies for the addition of electrons to the defect, are in very good agreement with the available experiments. Accordingly the electrons are more localized than in conventional dopants decaying in a radius of about 0.5 nanometers from the defect [8].

By mapping the ab initio DFT results in an extended Hubbard formalism, the resonant tunneling in an array of Ge-V_n complexes in silicon is analyzed in order to shed light on the transport mechanisms observed in the experimental I-V curves.

This strongly correlated system is characterized by very large on-site repulsion U and small electronic hopping t (U/t 250) and can be a platform to

study the Mott transition and the antiferromagnetic correlation at half filling. This study is part of a joined theoretical and experimental project funded by the Horizon 2020 European Funding Programme [9].

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