Ab initio analysis of close to surface divacancies in 3C-SiC

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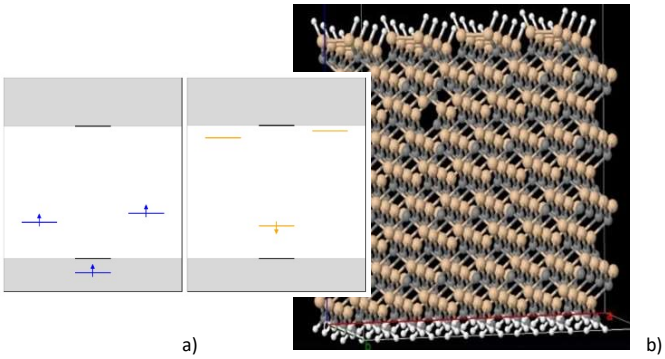
Abstract: The present study employs density functional theory to investigate multiple properties of neutral divacancies $V_{Si}V_C$ close to H terminated surface in cubic silicon carbide, a promising system for use in quantum sensing and simulations.

In order to undertake the ab-initio analysis of the near-surface defects state in cubic silicon carbide 3C-SiC, the (2x1):H surface reconstruction of the (001) surface has been selected. In the considered slab model, as illustrated in the Figure (Fig. 1), containing 670 atoms, the bottom C atoms were H saturated and the bottom layer was partially fixed, in the relaxation of atomic coordinates, to mimic the geometry of the bulk structure.



a) b)

Fig. 1 a) Electronic structure of spin defect positioned at ~6 Å from reconstructed Si-rich surface. The withe region corresponds to the computed 3C-SiC energy gap. b) Optimized geometry of the (2×1):H slab model obtained using a vacuum length comparable to the slab thickness.

The electronic structure of the spin defect and the relaxed geometry of the supercell were determined at the DFT level, using plane wave basis sets and Optimized Norm-Conserving Vanderbilt (ONCV) pseudopotentials, by means of Quantum Espresso package, for axial symmetric configuration of the neutral divacancy at different distances from the reconstructed Si-rich surface. It is noteworthy that the PBE exchange-correlation functional was employed in all calculations. Some obtained results are consistent with similar computational studies, on the same system, reported in literature [1].

Starting from the optimized geometries of the slabs, calculations of hyperfine couplings between the electronic and nuclear spin were carried out at the same level of theory, but using norm-conserving pseudopotentials with GIPAW reconstruction, by means of the GIPAW module of Quantum Espresso. The decoherence of point defect qubits is often governed by the electron spin-nuclear spin hyperfine interaction, that can be parameterized by using *first principles* calculations. Preliminary results obtained at the DFT level show values approximately one order of magnitude larger for the components of the hyperfine coupling tensors than the corresponding components obtained according to a semiclassical approach.

Finally, to understand the influence of the surface, the components *D* and *E* of the zero-field splitting (ZFS) tensor were computed. As expected, a certain sensitivity of the transversal component *E* of ZFS tensor to the position of the divacancy, relative to the surface, was found.

References

[1] Yizhi Zhu, Victor Wen-zhe Yu, and Giulia Galli, "First-Principles Investigation of Near-Surface Divacancies in Silicon Carbide" Nano Lett. **23**, 11453 (2023).