Spin-orbit and Jahn-Teller effect in split-vacancy impurity defects of diamond

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The success and limitations of NV centre of diamond induced a lot of interest towards new alternative point defects in semiconductors for quantum applications. Thus, identification of new point defects or theoretical prediction of physical parameters of identified ones has gained a lot of attention in the recent years. For example, it is already well established to use density functional theory (DFT) to predict the the hyperfine parameters for EPR, determine optical excitation energies or formation energies for defects. In my talk, I will go beyond the traditional methods of ab-inito calculations. We will present novel schemes to determine and characterize the electron-phonon interaction induced Jahn-Teller effect and spin-orbit coupling that governs various trigonal defect centres of diamond and compare our theoretical results with experimentally known data.

The fine structure of optical centres – splitting of their zero phonon lines (ZPL) – is usually attributed to the spin-orbit coupling. We will show that the Jahn-Teller and spin-orbit interactions must be treated simultaneously in SiV(-), GeV(-), SnV(-), PbV(-) centres of diamond to obtain quantitatively correct λ spin-orbit parameters in agreement with the experimental data [1]. Additionally, we identify [2] the NiV(-) system as the 1.4-eV optical ZPL by simulating its (λ) fine structure and other properties and thus, correct its previous assignment as the NE4 or 1.72-eV nickel related centre. On the other hand, two Jahn-Teller unstable holes adjointly culminate as an exemplary product Jahn-Teller $(e_g \otimes e_u) \otimes E_g$ system [3] in SiV(0), GeV(0), SnV(0), PbV(0) centres and it is responsible for the anomalous optical properties of the experimentally known 1.31-eV optical signal of SiV(0) in diamond.

In summary, we will show that ab-initio DFT provides an appropriate tool to obtain the parameters for various model Hamiltonians that are used to simulate experimentally observed (EPR, optical) spectra of defect centres in semiconductors.

[1] G. Thiering and A. Gali, Phys. Rev. X, 8, 021063 (2018).
[2] G. Thiering and A. Gali, Phys. Rev. Research, 3, 043052 (2021).
[3] G. Thiering and A. Gali, npj Computational Materials 5 (1), 18 (2018).