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Pd.D. subject : Modelling point defects for quantum application including electron-lattice interaction and surface effect

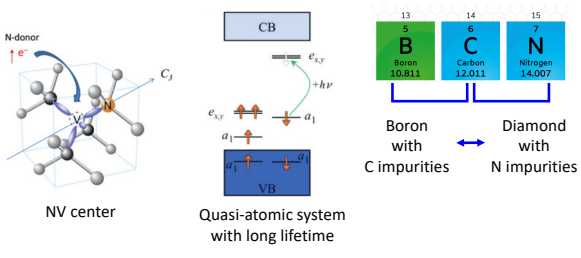
The rise of room-temperature applications - nanoscale magnetometry, thermometry, single photon emission, solid-state implementation of qubits - of the negatively charged nitrogen-vacancy NV^- center in diamond has motivated a renewed interest in the search, with theoretical methods, of other point defects - in diamond in another material- with a desired property for quantum application, e.g. a bright photoluminescence and a long coherence time of the spin ground state.

However, the fact that the local atomic structure of the defect ground-state or of the excited states is hardly accessible with direct experimental techniques prevents a direct understanding of the thermodynamics stability of defect charge states in the bulk, and of the expected quantum property. This makes the on-demand control of the defect charge state challenging, a problem even more complex near to the surface, because band bending induces a surface modification of the charge state and surface states of ubiquitous defects may be present.

In this Ph.D. work, theoretical methods will be used to predict the defect charge states and explore the effect of the proximity of the surface on the thermodynamic stability and on the spin structure. The objective is threefold: To apply the theoretical framework developed at LSI and predict the defect charge states in bulk; To study changes in the charge state brought by the proximity of the surface; To extend the Hubbard model used to compute the excited states and to account for the electron-lattice interaction in order to compute the zero-phonon line also for the excited states that cannot be predicted by the DFT only. Materials under considerations are carbides -diamond and silicon carbide- and borides - elemental boron and boron compounds. The theoretical method will rely on the Hubbard model developed at LSI in collaboration with IMPMC, and density functional theory (DFT) calculations.

Spin defects for quantum technologies

In 2D materials: hBN, TMDs (ex. WS_2, $MoSe_2$)
In 3D materials: Diamond[1], SiC



NV center

Quasi-atomic system with long lifetime

Properties near to the surface?

[1]A. Gali, *Nanophotonics* **8**, 1907 (2019).