Ab-initio theoretical study of NV-centers in diamane

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Abstract
Recent advances in quantum technologies have led to quantum computers that surpass classical computation limits [1]. Transmons, using superconducting loops, are the main qubit technology but require constant cryogenic cooling and have issues with noise sensitivity and scalability [2]. An alternative is to use negatively charged NV-centers in diamond lattices [3] where replacing a nitrogen atom next to a vacancy creates a two-level quantum system within the band gap, possibly acting as qubits, with transitions between bright and dark exciton states tunable by electromagnetic fields [4, 5]. Two-dimensional semiconductors may be even better hosts for NV-centers due to more isolated defects, higher radiative rates, and smaller Bohr effective radii [6, 7]. This work aims at studying theoretically diamanes, a 2D version of diamond (see. Fig. below) built form hydrogenated few-layers of graphene [8, 9, 10]. In last years, several evidence of partial hydrogenation of such systems with a soft approach have been proposed by some of our close collaborators [11, 12]. Optically, diamanes have direct, wide band gap at the Γ point and shows a decrease of the fundamental gap value as function of graphene layer numbers, a behaviour that will be discussed. Furthermore, the electronic dispersion including NV-centers shows the emergence of different localized states within the band gap at the Γ point, there details will be presented.

References

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Figures

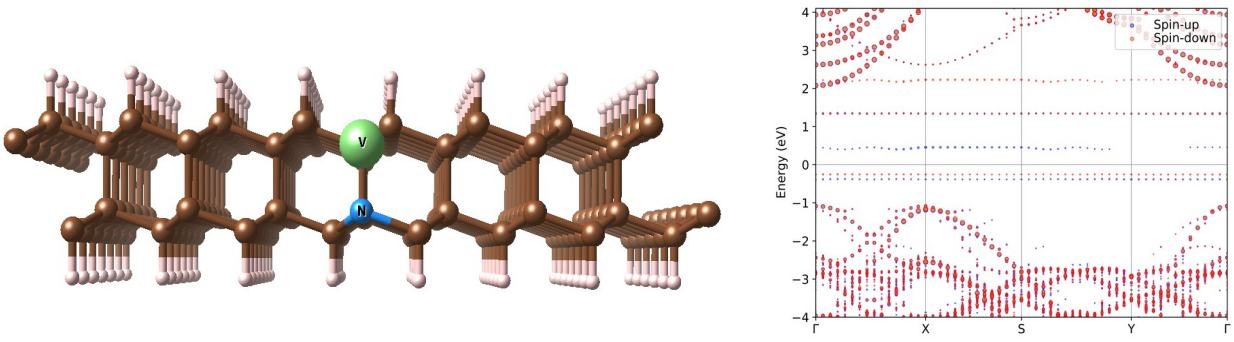

Figure 1: Side view of NV-center in bi-layer diamane lattice and its band structure, H, C and N atoms are represented in pink, brown and blue respectively while green is for the vacancy.