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First principles characterization of nitrogen dopant-vacancy complexes in graphane

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We compute first principles calculations to characterize four types of point defects in the 2-dimensional material graphane. The point defects we consider in this contribution are nitrogen dopant-vacancy complexes and their various charge states. We compute the formation energies, binding energies, U-parameters and other electronic properties of these impurity-vacancy complexes in graphane monolayer with the objectives of utilising this group of point defects for quantum computing. Analysis of DOS plots and defect level diagrams shows that the complex formed by a nitrogen dopant substituting a carbon atom adjacent to a hydrogen vacancy exhibit interesting properties that may make this point defect complex a possible qubit candidate. Charge neutrality pins the fermi level at a value close to 2eV deep between the VBM and the CBM making this complex a deep centre defect.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

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