Defect Processes in Hexagonal Boron Nitride for Application in Quantum Technologies

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Quantum computers have emerged as one of the most promising alternative technologies, as they have the potential to solve problems which will always be intractable for classical computers. Applications range from breaking public-key cryptography to novel drug discovery. At the heart of this advancement in hardware, materials are playing a crucial role. Many candidates have been proposed as qubits, with most of them operating at very low temperatures. However, their efficiency is limited by their environmental requirements, which remains a major block to scaling-up of quantum technologies. Several attempts have been made to address this issue, with solid state spin qubits based on defect centres in wide bandgap semiconductors being a promising solution that could lead to devices operating at room temperature. Hexagonal boron nitride (hBN) is one such semiconductor that can be used as a spin-defect host as it has excellent chemical and thermal stability, a wide band gap, and the presence of stable optically active defects with a broad emission range. Certain intrinsic point defects within hBN have been suggested to be suitable for quantum technologies, in particular the negatively charged boron vacancy (V_B^{-1}) [1]. Herein, we apply density functional theory calculations to study the electronic properties of various charge states of the intrinsic defects in bulk hBN. Calculating the defect formation energies of vacancies, substitutions and interstitials as well as their density of states, we found that boron interstitials, which are essentially intercalated given the layered nature of hBN, exhibit deep level states, suitable for optical transitions in quantum technologies. Furthermore, we demonstrate that the zero-phonon line (ZPL) energy for B_i^{-2} is predicted at 0.98 eV, falling within the desirable telecom range for spin defects. The present work underscores the significance of intrinsic defects in bulk hBN for quantum technologies, emphasizing opportunities for advancements from single photon emission to quantum sensing.

[1] R. Rizzato, M. Schalk, S. Mohr, et al., ”Extending the coherence of spin defects in hBN enables advanced qubit control and quantum sensing”, Nat Commun 14, 5089 (2023)