

# Native point defects and impurities in hexagonal boron nitride

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Recently hexagonal boron nitride (h-BN) has attracted a lot of attention because of discovery of single-photon emitters (SPEs) in monolayer, multi-layer and bulk [1–4]. Single photon emission exhibits linear optical polarization and has been attributed to point defects. These results highlight the potential of h-BN for applications related to quantum information science, including quantum computing and quantum-secure communication. Despite active investigations, the nature of these emitters has so far remain unresolved [5–6].

We study the properties of native defects and impurities in h-BN using density functional theory with a hybrid functional. We also investigate the migration properties of these point defects to determine their kinetics at different temperatures. Native vacancy and antisite defects have high formation energies, and are unlikely to form under thermodynamic equilibrium for typical growth conditions. Self-interstitials can have low formation energies when the Fermi level is near the band edges, and may form as charge compensating centers; however, their low migration barriers render them highly mobile, and they are unlikely to be present as isolated defects.

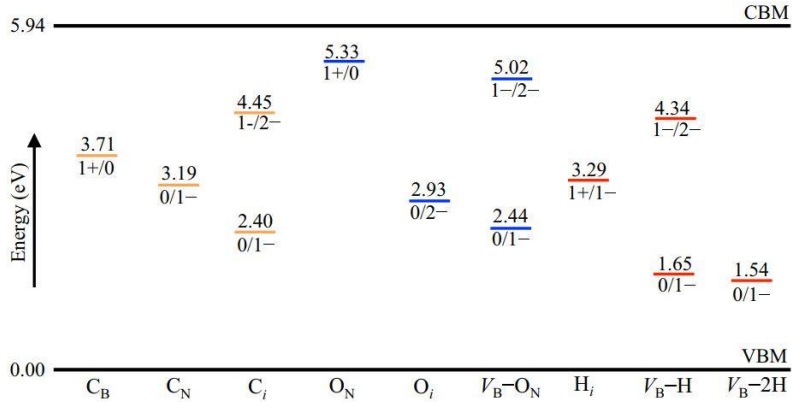


FIG. 1: . Charge-state transition levels for impurity-related defect species in h-BN. Defect levels related to C are shown in orange, due to oxygen in blue, and hydrogen in red [7].

The defect chemistry of h-BN is most likely dominated by defects involving carbon, oxygen, and hydrogen impurities. Substitutional carbon and oxygen, as well as interstitial hydrogen and boron vacancy-hydrogen complexes, are low-energy defects in h-BN. Based on our results, we can rule out several proposed sources for defect-related luminescence in h-BN [7]. In particular, we find that the frequently observed 4.1 eV emission cannot be associated with recombination at CN, as has been commonly assumed. We discuss possible defect origins for the recently observed single-photon emission in h-BN, identifying interstitials or their complexes as plausible centers.

- [1] T. T. Tran, K. Bray, M. J. Ford, M. Toth, and I. Aharonovich, *Nat. Nanotechnol.* 11, 37 (2016).
- [2] T. T. Tran, C. Zachreson, A. M. Berhane, K. Bray, R. G. Sandstrom, L. H. Li, T. Taniguchi, K. Watanabe, I. Aharonovich, and M. Toth, *Phys. Rev. Appl.* 5, 034005 (2016).
- [3] Z. Shotan, H. Jayakumar, C. R. Conside, M. Macko, H. Fedder, J. Wrachtrup, A. Alkauskas, M. W. Doherty, V. M. Menon, and C. A. Meriles, *ACS Photonics* 3, 2490 (2016).
- [4] A. L. Exarhos, D. A. Hopper, R. R. Grote, A. Alkauskas, and L. C. Bassett, *ACS Nano* 11, 3328 (2017).
- [5] S. A. Tawfik, S. Ali, M. Fronzi, M. Kianinia, T. T. Tran, C. Stampfl, I. Aharonovich, M. Toth, and M. J. Ford, *Nanoscale* 9, 13575 (2017).
- [6] F. Wu, A. Galatas, R. Sundararaman, D. Rocca, and Y. Ping, *Phys. Rev. Materials* 1, 071001 (2017).
- [7] L. Weston, D. Wickramaratne, M. Macko, A. Alkauskas, and C. G. Van de Walle, *Phys. Rev. B* **97**, 214104 (2018).