Defects in semi-conductors for Quantum Applications

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Abstract

Discovery of single photon emission (SPE) [1] from 2D materials has opened a new arena of research because of the unique electric, magnetic and optical properties possessed by these SPE's. Strong luminescence owing to the close proximity of emitters to the surface (contrary to 3D semiconductors) makes them superior for applications in high quantum efficiency applications. Hexagonal boron nitride (h-BN) is one such wide bandgap 2D semiconductor material, which has become very popular recently due to the observation of room temperature single photon emission (SPE) in both the visible and UV regions. SPE'S in h-BN possess room-temperature operation, ultra-high brightness, full polarization, and tuneable emission [2] making them very interesting for quantum sensing and optical communications. Based on these properties such systems provide very attractive platform that can help to realize, control, manipulate and measure individual quantum states. The defect systems with similar properties must be explored in other 2D materials, as this will broaden the range of materials available for such applications, consequently revolutionising this field. In the present work we have shortlisted/ the defect systems with optimal properties for various quantum applications e.g. qubits, quantum key distribution, brain magnetometers etc., based on our screening study of intrinsic point defects in dynamically and thermodynamically stable and non-magnetic host systems from C2DB database [3]. We study various aspects and properties of these defect systems e.g. photoluminescence (PL) line shape, Transition dipole moment, Radiative recombination rates, Inter-system crossing rates, Hyperfine coupling parameters, Zero field splitting, Spin-Coherence times etc. We identify a set of defect systems, with ideal properties, which can be exploited for various quantum technologies.

References

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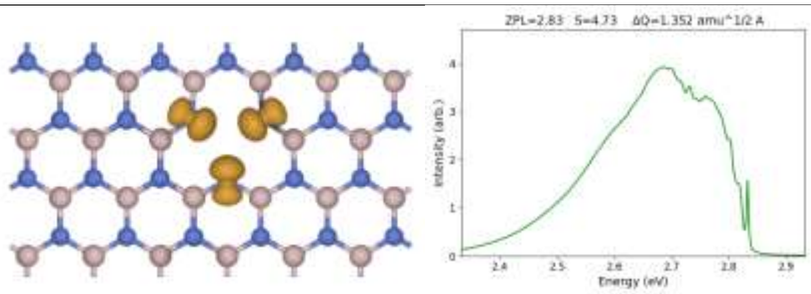
Figures



(a) (b)

Figure 1: (a) The Iso-surface of the calculated spin-density (isovalue of 0.002|e|/Å^3) for V_B^{-1} defect in hexagonal boronnitride (b) The calculated PL line shape for the HOMO to LUMO transition in the spin-up channel for SiCH2_Si_H defect in -1 charge state.