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Defect States in Hexagonal Boron Nitride: Assignments of Observed Properties and Prediction of Properties Relevant to Quantum Computation

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Key properties of 9 possible defect sites in hexagonal boronitride (h-BN), V_N, V_N^{-1}, C_N, V_NO_{2B}, V_NN_B, V_NC_B, V_BC_N, $V_BC_NSi_N$, and $V_NC_BSi_B$, are predicted using density-functional theory (DFT) corrected applying results from high-level *ab initio* calculations. Observed h-BN electron-paramagnetic resonance (EPR) signals at 22.4 MHz, 20.83 MHz, and 352.70 MHz are assigned to V_N, C_N, and V_NO_{2B}, respectively, while the observed photoemission at 1.95 eV is assigned to V_NC_B. Detailed consideration of the available excited states, allowed spin-orbit couplings, zero-field splitting, and optical transitions is made for somewhat analogous defects V_NC_B and V_BC_N. Long-living quantum memory in h-BN can be achieved for V_NC_B owing to the lifetime differences of first and second order transitions from different triplet sub-states to the singlet ground state as is seen for N_2V defect in diamond. While V_BC_N is predicted to have a triplet ground state, and for it spin-polarization by optical means is predicted to be feasible while suitable optical excitations are also identified, making this defect of interest for possible quantum-qubit operations.

Biography:

Sajid Ali is a 3rd year PhD student at *University of Technology Sydney, Ultimo, New South Wales 2007, Australia*. He is also a lecturer in physics at *GC University Faisalabad, Pakistan.* He has over 15 publications that have been cited over 100 times.