A. Sajid et al., J Material Sci Eng 2018, Volume 7
DOI: 10.4172/2169-0022-C8-113

19th World Congress on

Materials Science and Engineering

June 11-13, 2018 | Barcelona, Spain

Defect states in hexagonal boron nitride: Assignments of observed properties and prediction of properties relevant to quantum computation

A. Sajid[2], **Jeffrey R. Reimers**[1] and **Michael J. Ford**[1]
[1]University of Technology Sydney, Australia
[2]GC University, Pakistan

Hexagonal boron nitride (h-BN) is a wide band gap (~6 eV) 2-dimensional (2-D) material with the potential to host many such colour centres [1-8] that are promising candidates for quantum applications. Defects can dramatically alter the electronic and magnetic properties of the host Semiconductor. While both nitrogen (Nv) and boron (Bv) vacancies can act as paramagnetic centres in h-BN [9], electron paramagnetic resonance (EPR) studies indicate that Nv are more important [10-15]. Two types of paramagnetic centres have been identified: (i) three-boron centres (TBC) in which an unpaired electron interacts with three equivalent boron (B^{11}) nuclei, producing 10-line EPR spectra, and (ii) one-boron centres (OBC) in which an unpaired electron interact with only a single B^{11}, producing 4-line EPR spectra. A-priori calculations using density-functional theory (DFT) can provide useful tools for the interpretation of EPR by comparing the experimental and calculated hyperfine constants [16-20]. We consider detailed models of the TBC and OBC defects in h-BN, as well as proposing many new defect centres, particularly defects involving introduced carbon impurity atoms one's which are thought of being responsible for single photon emission in hBN. We do Group-theoretical analysis to suggest new directions for experimental studies. 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) that are corrected by applying results from high-level ab initio calculations. Detailed consideration of the available excited states, allowed spin-orbit couplings, zero-field splitting, and optical transitions is made for the two related defects V_NC_B(Fig.1.) and V_BC_N. We propose that ground-state spin polarization and long-lived quantum memory in h-BN can be achieved for V_BC_N and V_NC_B respectively.

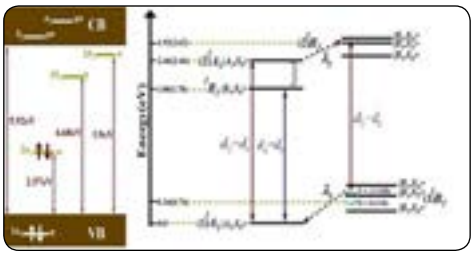

Figure 1: (a) Key DFT orbitals from the (1)1A1 closed-shell ground-state electronic structure of VNCB. The states are labelled according to the symmetry of Irreducible representation as per C2v point group. x(y,z)-axis are perpendicular(in the) to the plane of defect. (b) HSE06 adiabatic energies of low lying states of VNCB as calculated by DFT, with, in (), these energies corrected according to ab initio CCSD(T), EOMCCSD, and CASPT2 calculations for a model compound [23]. Allowed transition polarizations d, spin-orbit couplings driving non-radiative transitions and zero-field splittings are also indicated.

Recent Publications:

1. A. Sajid, J. R. Reimers, and M. J. Ford, Physical Review B 97, 064101 (2018).
2. J. Reimers, A. Sajid, R. Kobayashi, and M. Ford, Journal of chemical theory and computation (2018).
3. (A.Sajid, S. A. Tawfik)Equal Authors, M. Fronzi, M. Kianinia, T. T. Tran, C. Stampfl, I. Aharonovich, M. Toth, and M. J. Ford, Nanoscale (2017).
4. G. Grosso, H. Moon, B. Lienhard, A. Sajid, D. K. Efetov, M. M. Furchi, P. Jarillo-Herrero, M. J. Ford, I. Aharonovich, and D. Englund, Nature Communications 8, 705 (2017).
5. i. Zhu, L. L. C Lem, T. Nguyen, K. Fair, A. Sajid, M. J Ford1, M. R. Phillips1 and C. Ton-That Journal of Physics D: Applied Physics, 50(2017).

Biography

A. Sajid Ali has his expertise in DFT and quantum chemistry approaches for simulating the material properties. He also uses group theory analysis to study the defect induced properties of Materials. His recent(PhD) work is majorly focused on studying the mechanism of Quantum Emsission from Defects in Hexagonal Boron Nitride. He is currently a final year PhD student at University of Technology Sydney Australia. and has already published a number of papers in high quality journals.

Sajid.Ali@student.uts.edu.au

Notes: