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Point Defects in Materials: A Useful Technique for Quantum Technology

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Abstract

This work explores point defects in wide-band-gap semiconductors as qubits platforms for quantum technologies applications. A study of the NV center in diamond is included as a guide for the exploration of candidate defects in cubic boron nitride (c-BN). Four defects are investigated in c-BN: N_B^{+1}, $(V_B{-}V_N)^0$, $(V_B{-}C_B)^0$ and $(V_B{-}Si_B)^0$. Ab-initio simulations were performed to investigate the properties of defects.

Introduction

Point defects have emerged as a powerful tool for advancing knowledge and technology. Their influence extends to cutting-edge fields such as quantum technologies, enabling significant findings and driving remarkable scientific progress.

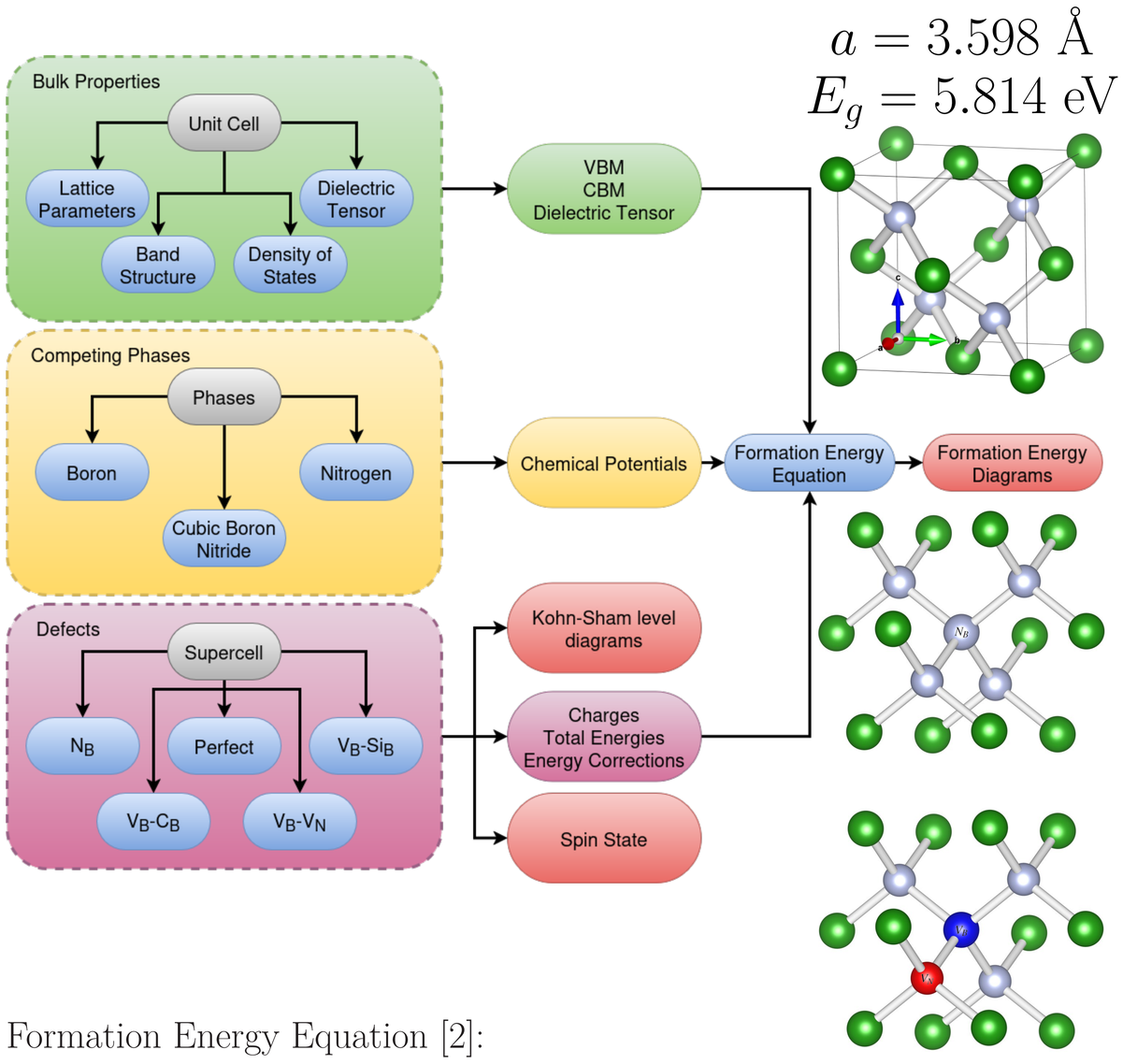
Requirements for Point Defect-Based Qubits [1]

A. The point defect must introduce energy levels within the band gap of the host material.
B. The energy levels must give rise to highly localized electronic states.
C. The highly localized states must be optically active.
D. The point defect must exhibit a paramagnetic ground state.
E. The spin state must exhibit long coherence times.

Methodology

Ab-initio calculations: Density Functional Theory

$a = 3.598$ Å
$E_g = 5.814$ eV

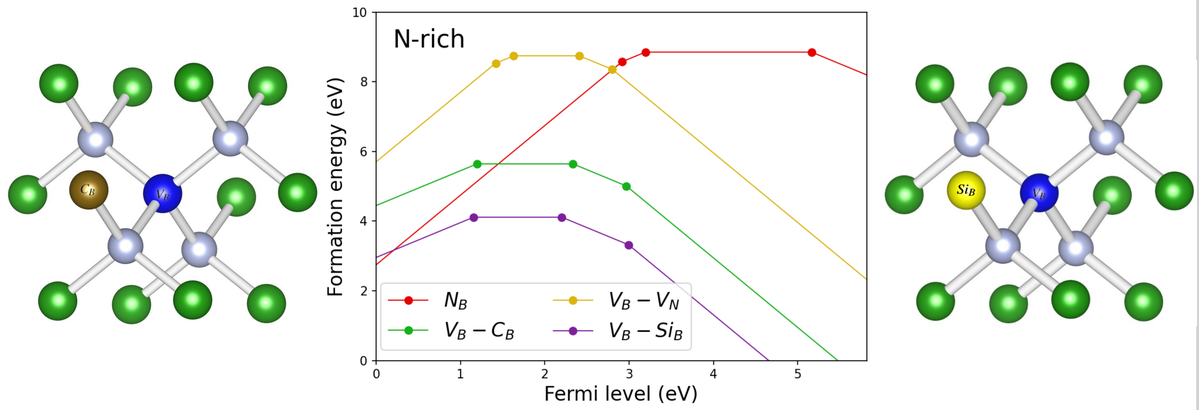


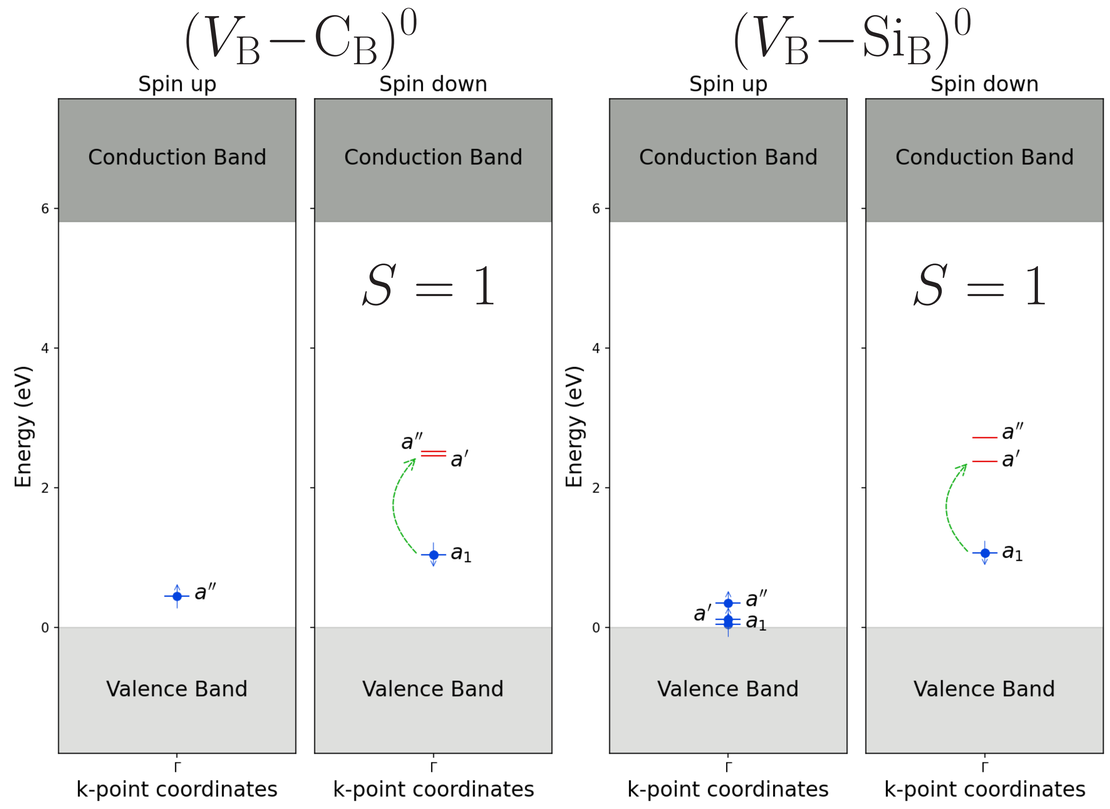
Formation Energy Equation [2]:

$$E^q_{form} = E^q_{def} - E_{perf} - \sum_i n_i \mu^*_i + q(E_{Fermi} + E_{VBM}) + E_{corr}$$

Results

Calculations with the HSE06 functional





Zero Phonon Line

- $(V_B{-}C_B)^0$: 0.933 eV ($\lambda = 1331$ nm)
- $(V_B{-}Si_B)^0$: 1.256 eV ($\lambda = 988$ nm)

Conclusions

Four point defects have been proposed as promising candidates:

- Only the native defect N_B^{+1} showed characteristics to act as a color center, emitting a wavelength of 757 nm.
- The $(V_B{-}V_N)^0$ defect emits at a telecom wavelength of 1503 nm (S-band).
- The $(V_B - C_B)^0$ emits at a telecom wavelength of 1331 nm (O-band).
- The $(V_B{-}Si_B)^0$ defect emits at a telecom wavelength of 988 nm.

References

J. R. Weber, W. F. Koehl, J. B. Varley, A. Janotti, B. B. Buckley, C. G. V. de Walle, and D. D. Awschalom, "Quantum computing with defects," *Proceedings of the National Academy of Sciences*, vol. 107, pp. 8513–8518, 2010.

A. Goyal, P. Gorai, H. Peng, S. Lany, and V. Stevanović, "A computational framework for automation of point defect calculations," *Computational Materials Science*, vol. 130, pp. 1–9, 2017.

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