Exploring point defects as qubit candidates in cubic boron nitride

Supervisors: Morten Hjorth-Jensen, Marianne Etzelmüller Bathen, Christopher Linderälv and David Rivas Gongora

Joseph P. Vera

Material Science of Semiconductors
University of Oslo

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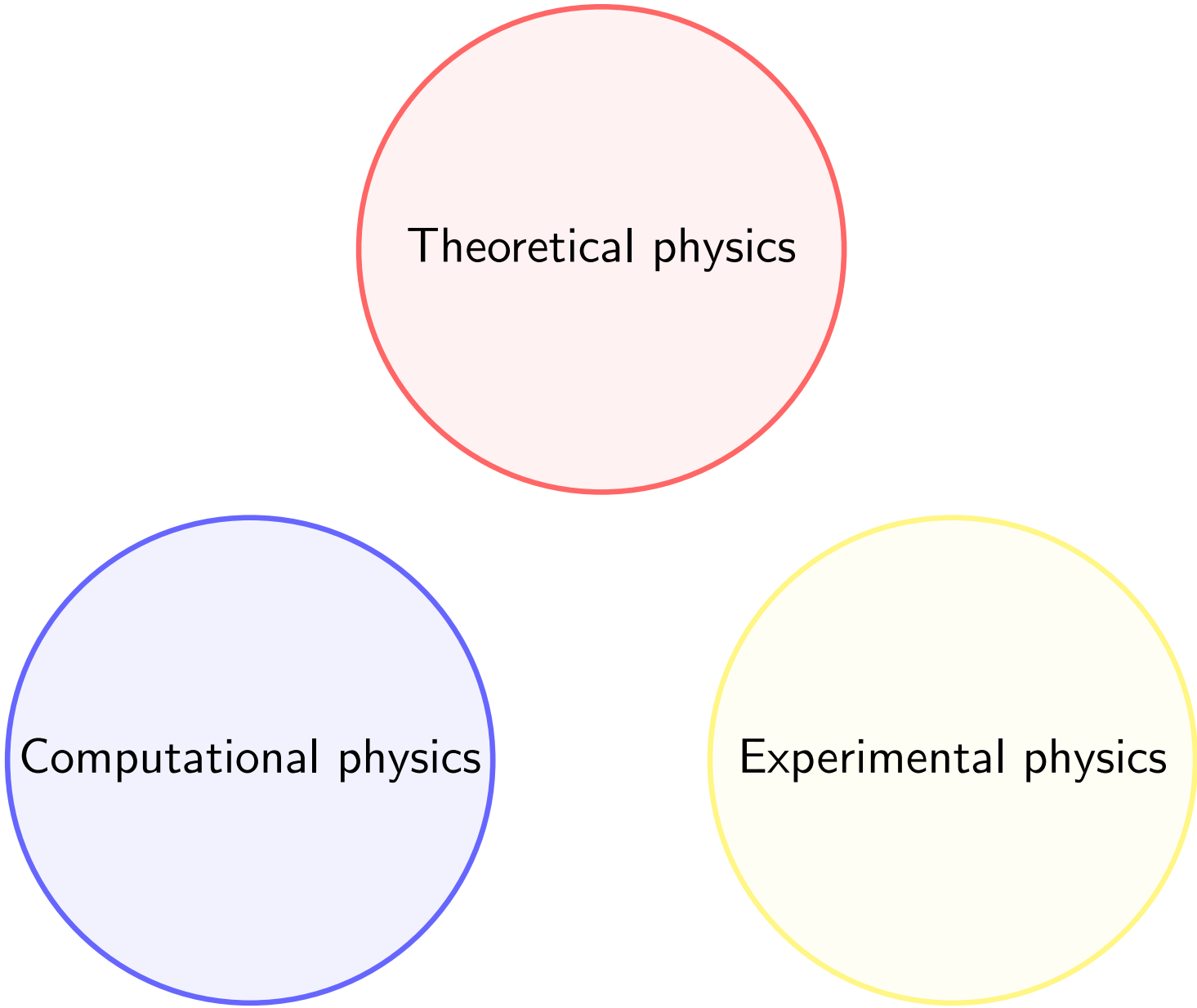
Theoretical physics
Computational physics
Experimental physics

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Predicting solid state material platforms for quantum technologies

Oliver Lerstøl Hebnes[1,2], Marianne Etzelmüller Bathen[3]✉, Øyvind Sigmundson Schøyen[2], Sebastian G. Winther-Larsen[2,4], Lasse Vines[5] and Morten Hjorth-Jensen[2,6]

Table 3. Material properties from the MP database.

Approach	Material	Crystal structure	MP code	Density (g cm^{-3})	Band gap (eV)	a, b, c (Å)	α, β, γ (∘)
Empirical approach to 0.85 confidence	CdSe	Hexagonal	mp-1070	5.3	0.6	4.4, 4.4, 7.2	90, 90, 120
	CuI	Hexagonal	mp-569346	5.8	1.2	4.3, 4.3, 7.0	90, 90, 120
	CuI	Cubic	mp-22895	5.8	1.2	4.3, 4.3, 4.3	60, 60, 60
	CdSe	Cubic	mp-2691	5.3	0.5	4.4, 4.4, 4.4	60, 60, 60
	BN	Cubic	mp-1639	3.5	4.6	2.6, 2.6, 2.6	60, 60, 60
	InAs	Cubic	mp-20305	5.3	0.3	4.4, 4.4, 4.4	60, 60, 60
	$ZnCd_3Se_4$	Cubic	mp-1078597	5.3	1.7	6.1, 6.1, 6.1	90, 90, 90
	BC_2N	Tetragonal	mp-1008523	3.3	1.6	2.6, 2.6, 3.7	90, 90, 90
	BC_2N	Orthorombic	mp-629458	3.4	1.8	2.5, 2.6, 3.6	90, 90, 90

Cubic Boron Nitride

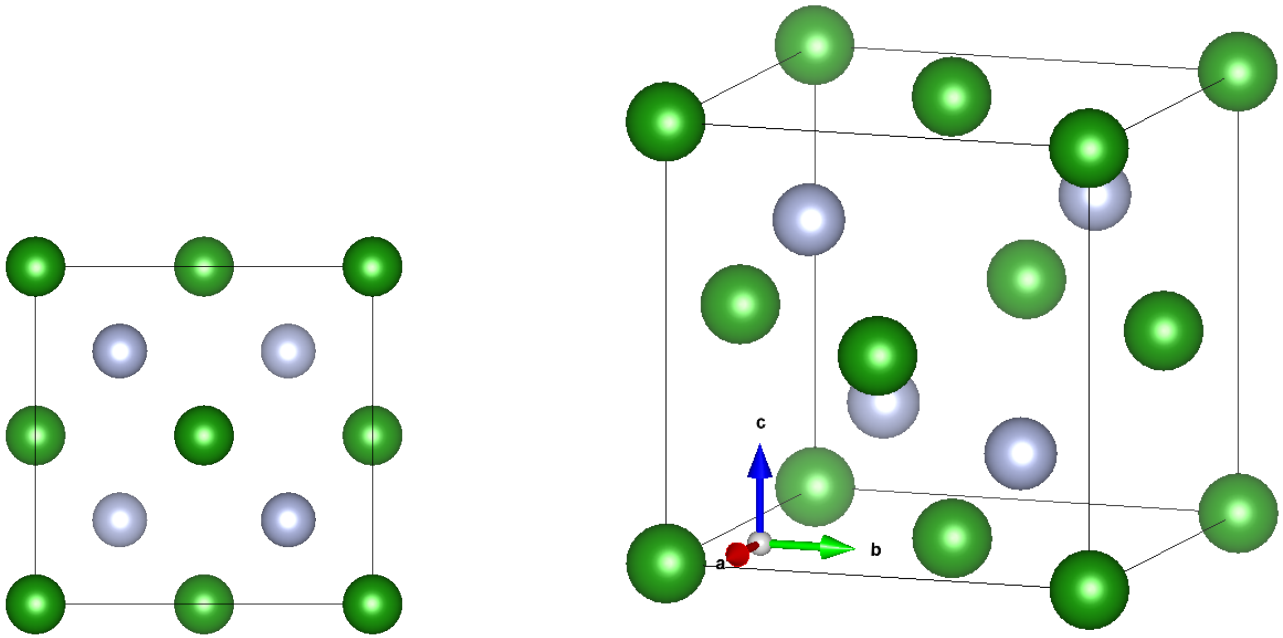
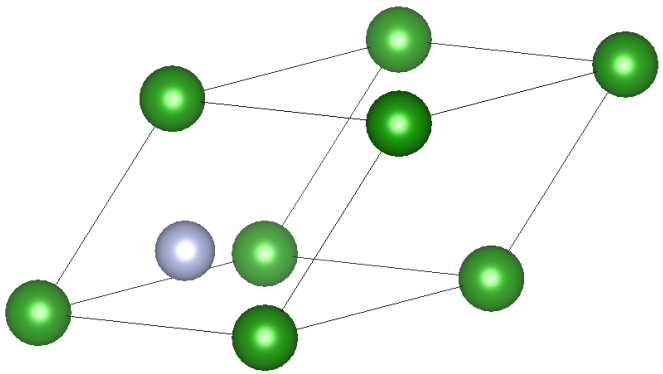


Table: Lattice parameters [1]

cell	Constants (Å)	Angles	Volume ($Å^3$)
	a=b=c	$\alpha = \beta = \gamma$	
Initial	a=3.630	$\alpha = 90°$	47.832
Final	a=3.626	$\alpha = 90°$	47.656

- Calculations of lattice parameters, band gap, density of states and band structure using GGA-PBE pseudopotential.

Initial test : Primitive cell



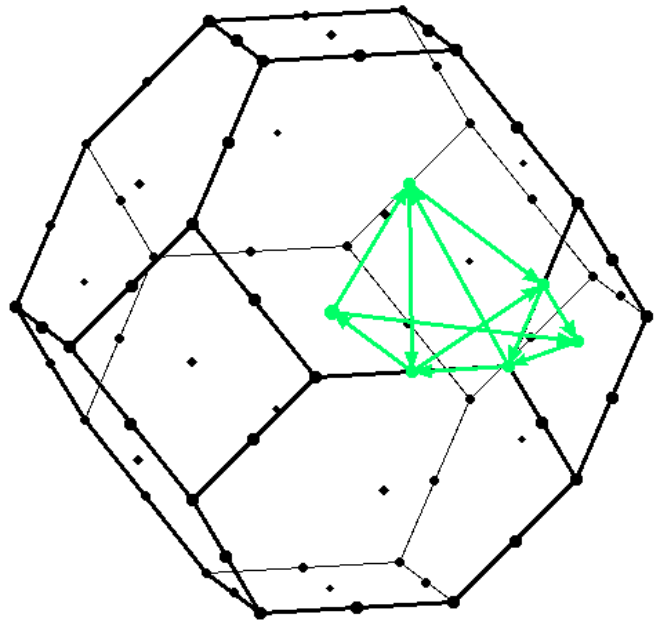
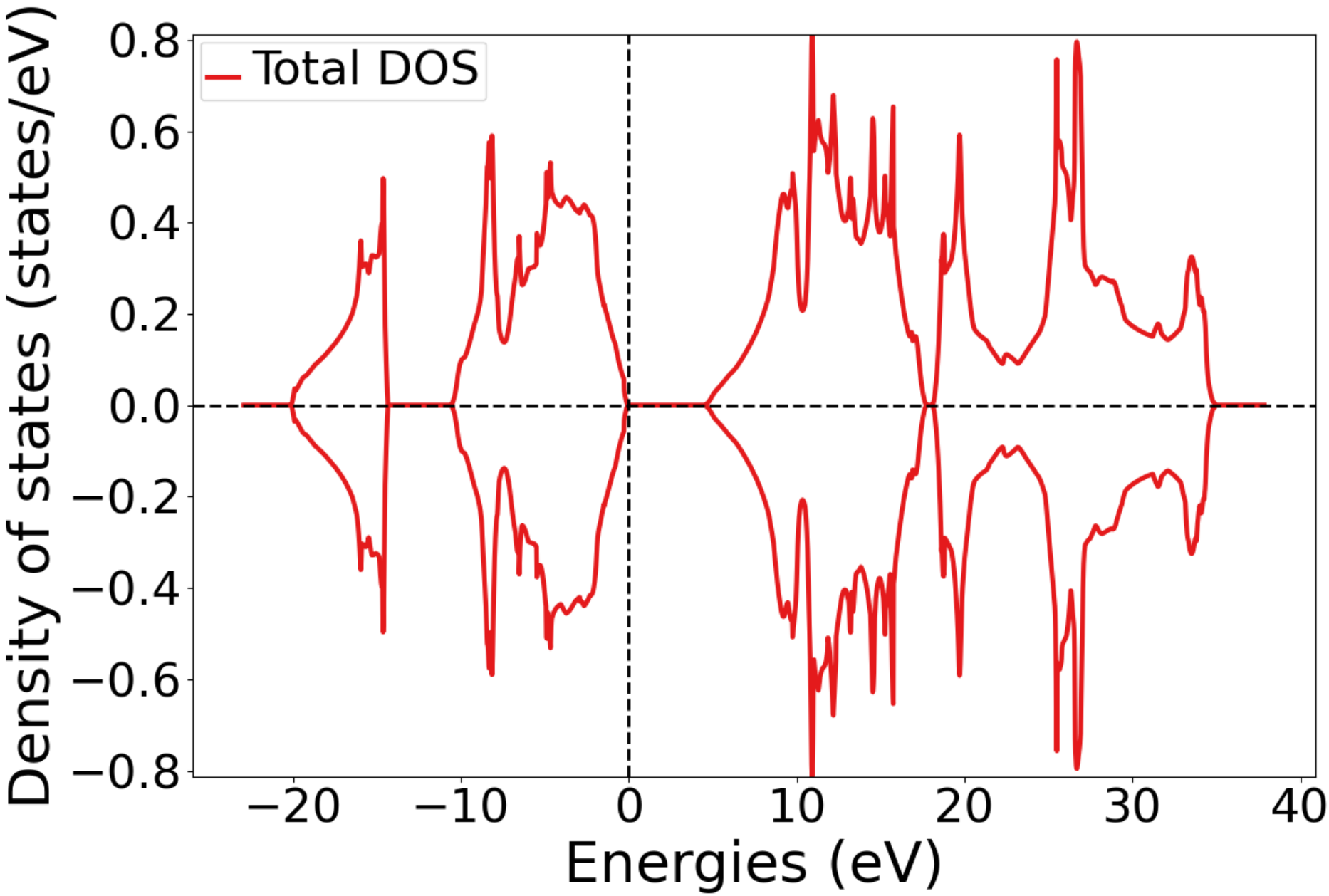
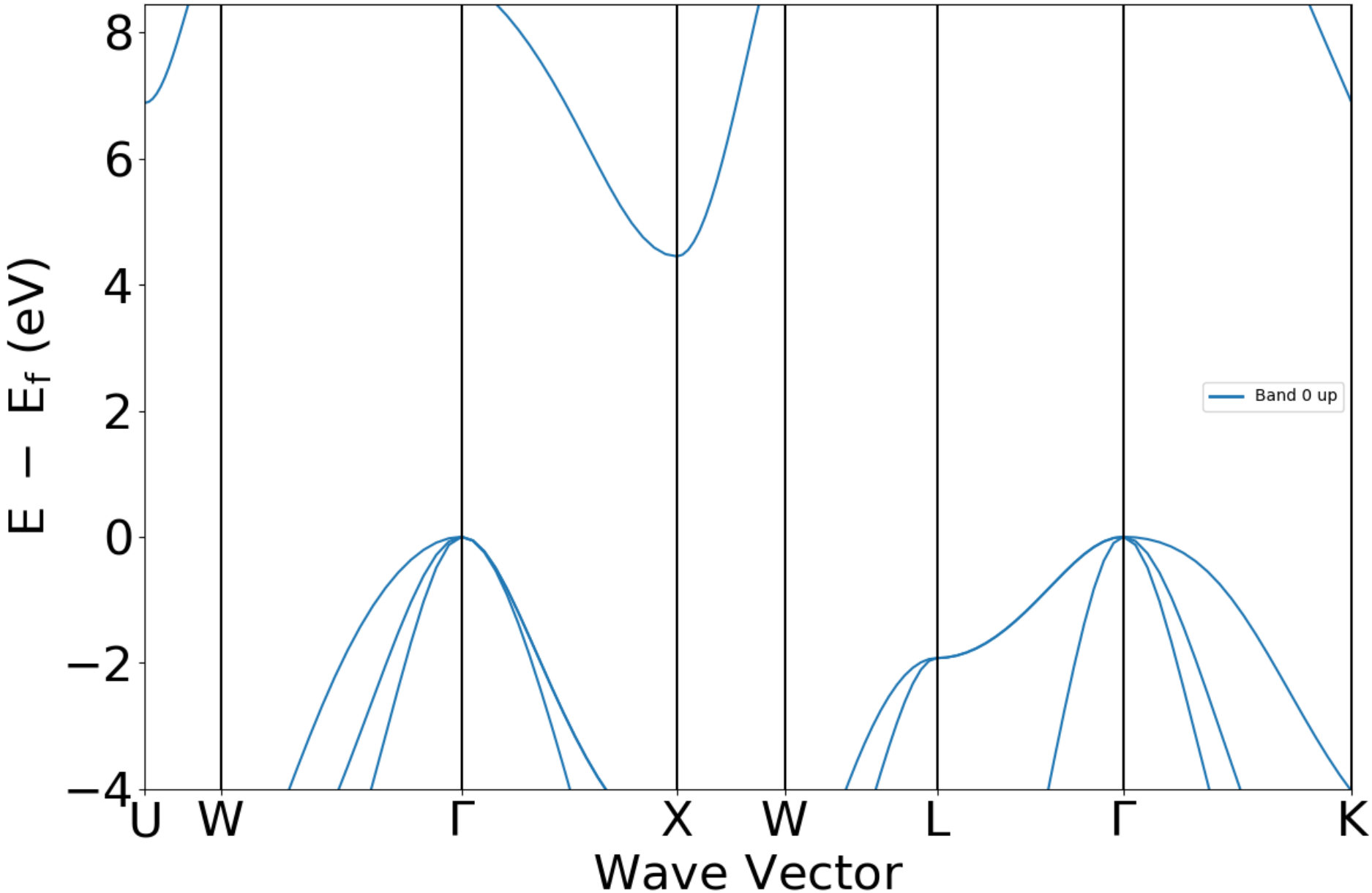
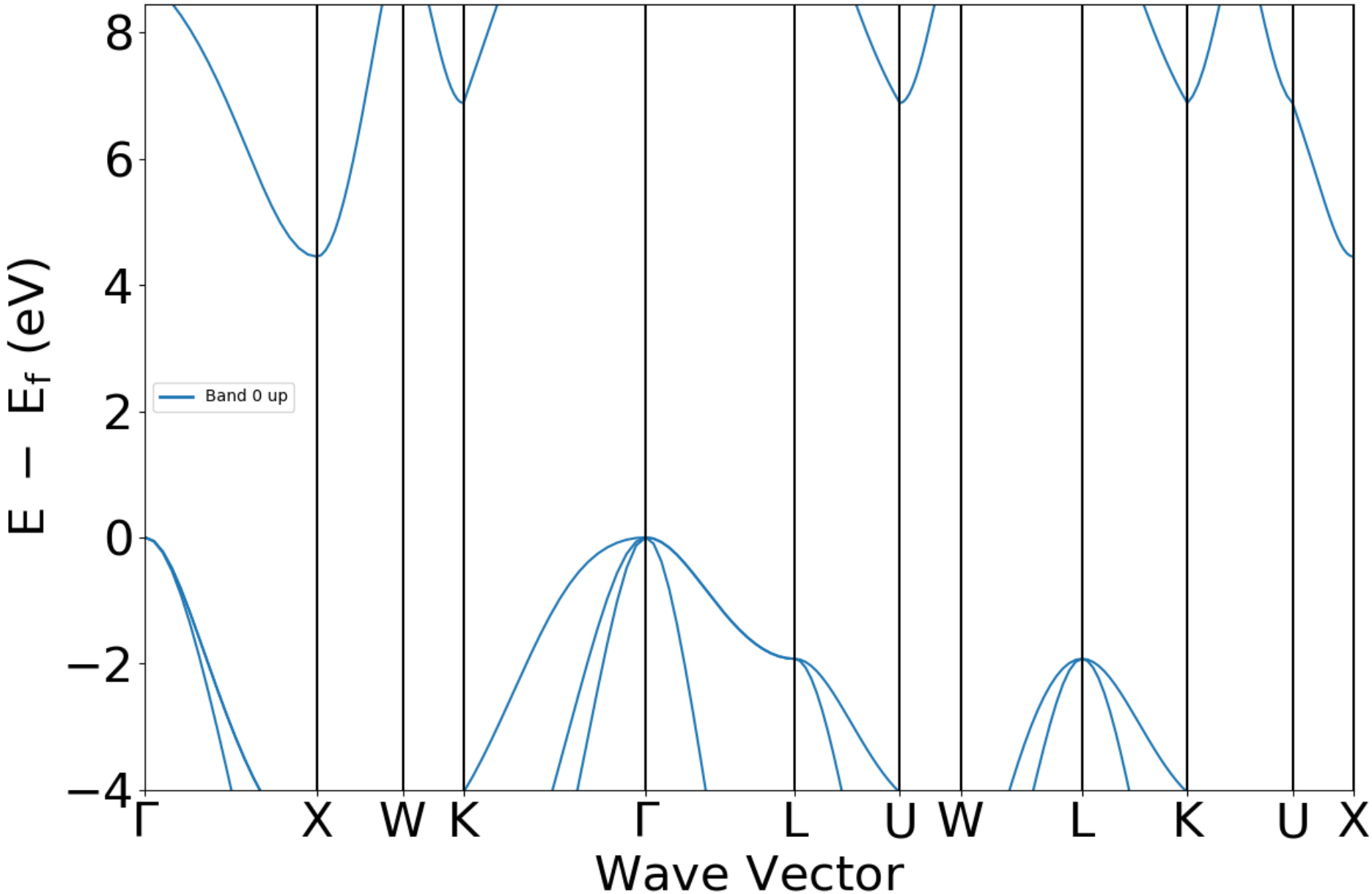


Table: Lattice parameters [1]

cell	Constants (Å)	Angles	Volume (Å^3)	Bandgap (eV)
	a=b=c	$\alpha = \beta = \gamma$		4.450
Initial	a=2.567	$\alpha = 60°$	11.958	
Final	a=2.564	$\alpha = 60°$	11.914	


Total DOS
Density of states (states/eV)
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
−0.8
−20
−10
0
10
20
30
40
Energies (eV)


8
6
4
2
0
−2
−4
E − E_f (eV)
U
W
Γ
X
W
L
Γ
K
Wave Vector
Band 0 up


8
6
4
2
0
−2
−4
E − E_f (eV)
Band 0 up
Γ
X
W
K
Γ
L
U
W
L
K
U
X
Wave Vector

- Calculations of band gap, density of states and band structure using HSE06 pseudopotential.

- Initial screening of multiple defect candidates based on available literature

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Energetics of carbon and oxygen impurities and their interaction with vacancies in cubic boron nitride

Walter Orellana[†]
Departamento de Física, ICEx, Universidade Federal de Minas Gerais, CP 702, 30123-970, Belo Horizonte, MG, Brazil

H. Chacham[*]
Department of Physics, University of Texas, Austin, Texas 78712

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We investigate, through first-principles calculations, the energetics of substitutional carbon and oxygen impurities as well as complexes involving these impurities and vacancies in cubic boron nitride (c-BN). The formation energies and the electronic and structural properties of these defects in their various charge states are investigated. We find that, under a boron-rich condition, both the carbon and the oxygen impurities at the nitrogen site (C_N and O_N) have formation energies comparable to or lower than those calculated for the vacancies, which are the lowest-energy intrinsic defects. Regarding defect complexes, we find that the donor character observed for the nitrogen vacancy (V_N) can be compensated by the C_N impurity in the formation of a V_N-C_N complex which has low formation energies. We also find that the V_B-O_N complex has low formation energies under n-type conditions. In contrast to the above mentioned complexes, we find that the V_B-C_B complex has high formation energies under a boron-rich condition, and shall only occur under a nitrogen-rich condition.

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Letter

Telecom-wavelength NV-center analogs in cubic boron nitride

Mark E. Turiansky [*] and Chris G. Van de Walle [†]
Materials Department, University of California, Santa Barbara, California 93106-5050, USA

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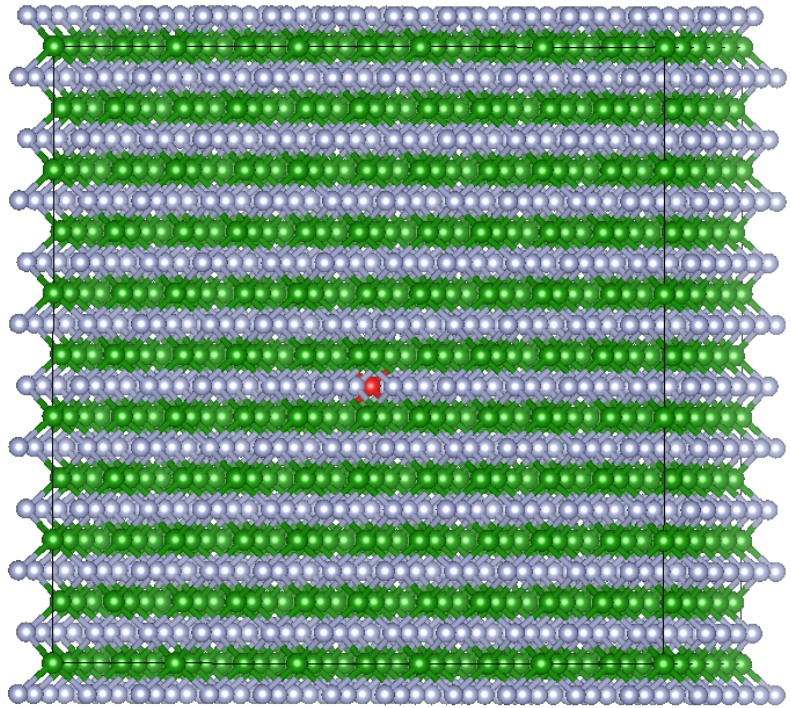
We apply first-principles calculations to investigate V_B-C_B and V_B-Si_B complexes in cubic boron nitride as potential quantum defects. We find that these centers possess a triplet ground-state spin, analogous to that of the prototype quantum defect, the NV center in diamond. In contrast, the main optical transition of these complexes occurs in the telecom O-band, making them appealing for quantum networking applications. Furthermore, the coupling to phonons is weaker than in the NV center, resulting in a much larger fraction of photons (22%) being emitted in the zero-phonon line. One inherent drawback of the longer emission wavelength is stronger nonradiative recombination; however, the resulting lower quantum efficiency can be mitigated by cavity coupling.

Calculations

- Defect stabilities
- Formation energy diagrams
- Zero-phonon line (ZPL) energies
- Spin states

- Selection of a few defects (2 - 4) to look at in further detail



Calculate defect properties

- Emission line shapes
- Spin coherence times
- Excited states
- Time-dependent properties (WEST)

- Experimental measurements using photoluminescence (PL) to explore defects

Phenomenon: single-photon emitters (SPE)

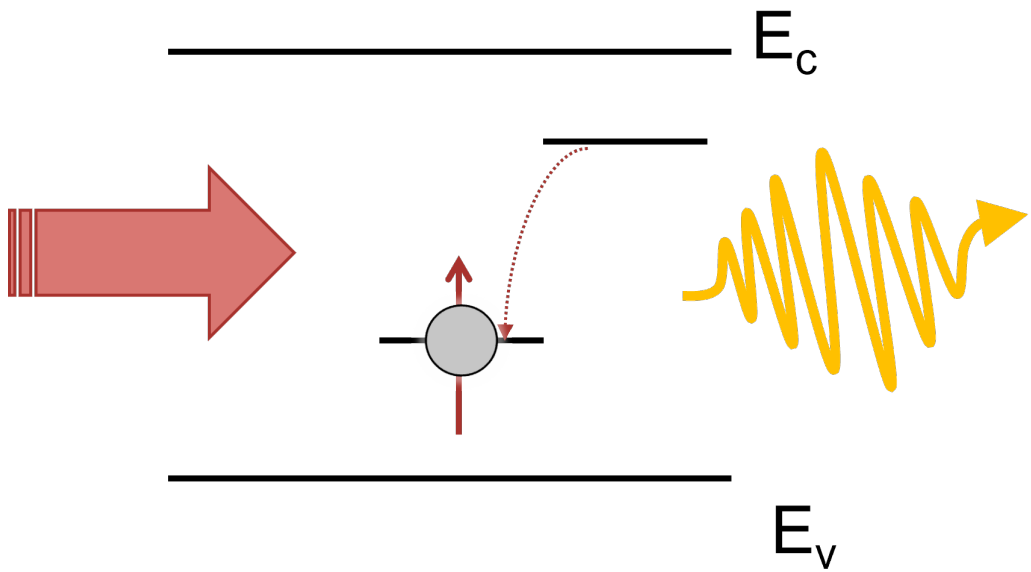


Figure: Courtesy to Marianne Etzelmüller Bathen

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- [1] https://next-gen.materialsproject.org/materials/mp-1639/.
- [2] Hebnes, O.L., Bathen, M.E.& Schøyen, Ø.S. (2022). Predicting solid state material platforms for quantum technologies. *npj Comput. Mater.*, 207(8), 1-15. DOI: 10.1038/s41524-022-00888-3.
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- [4] Turiansky, M.E. & Van de Walle, C.G. (2023). Telecom-wavelength NV-center analogs in cubic boron nitride. *Phys. Rev. B*, 108, L041102-1 - L041102-5. DOI: 10.1103/PhysRevB.108.L041102.