Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary Information: Band Gap and Electronic Structure of Ternary Nitride BP_3N_6: Experiment and Theory

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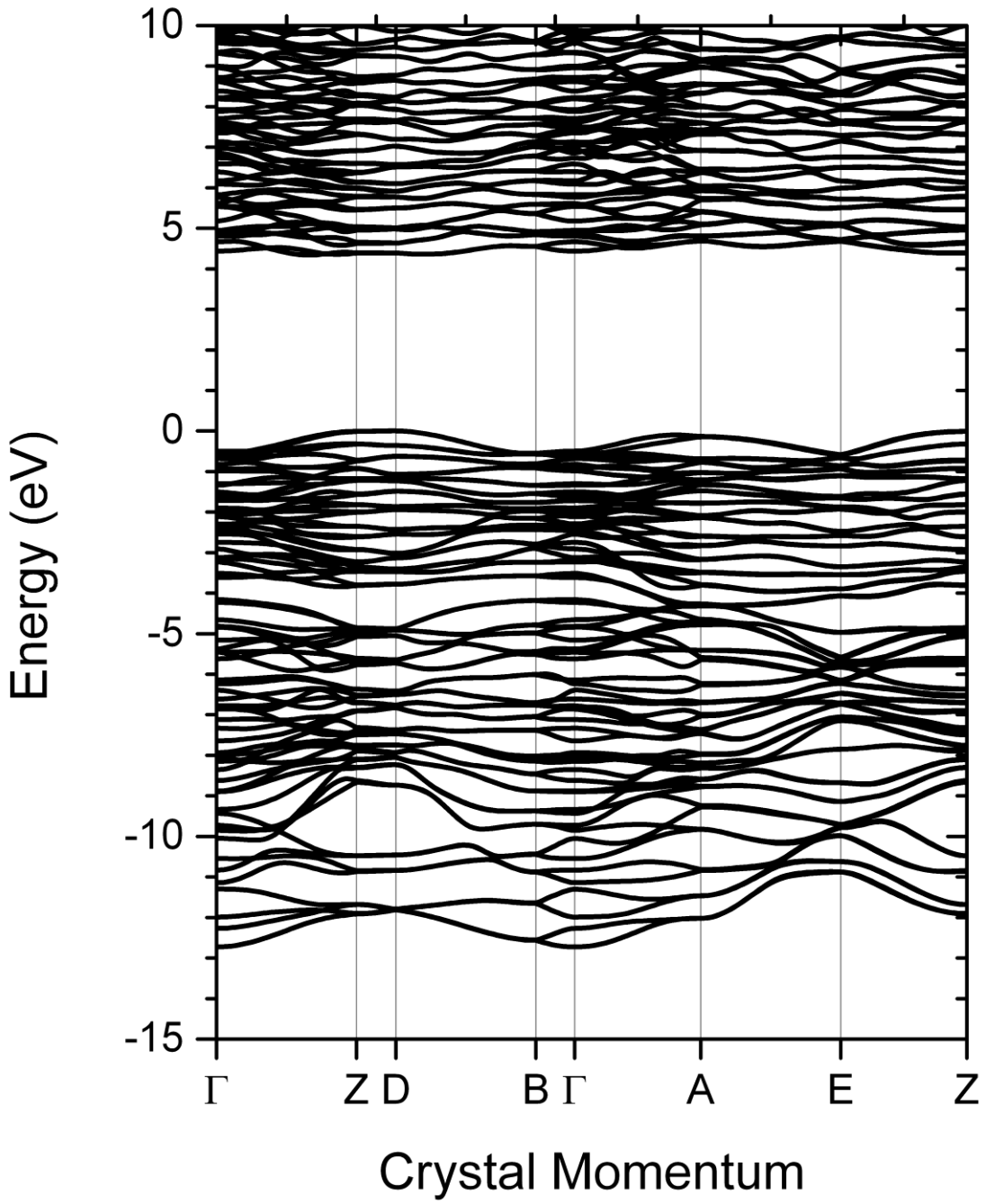

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Figure S1. Calculated band structure of BP_3N_6. The horizontal axis of the band structure panel corresponds to a path through high symmetry points in the Brillouin zone.

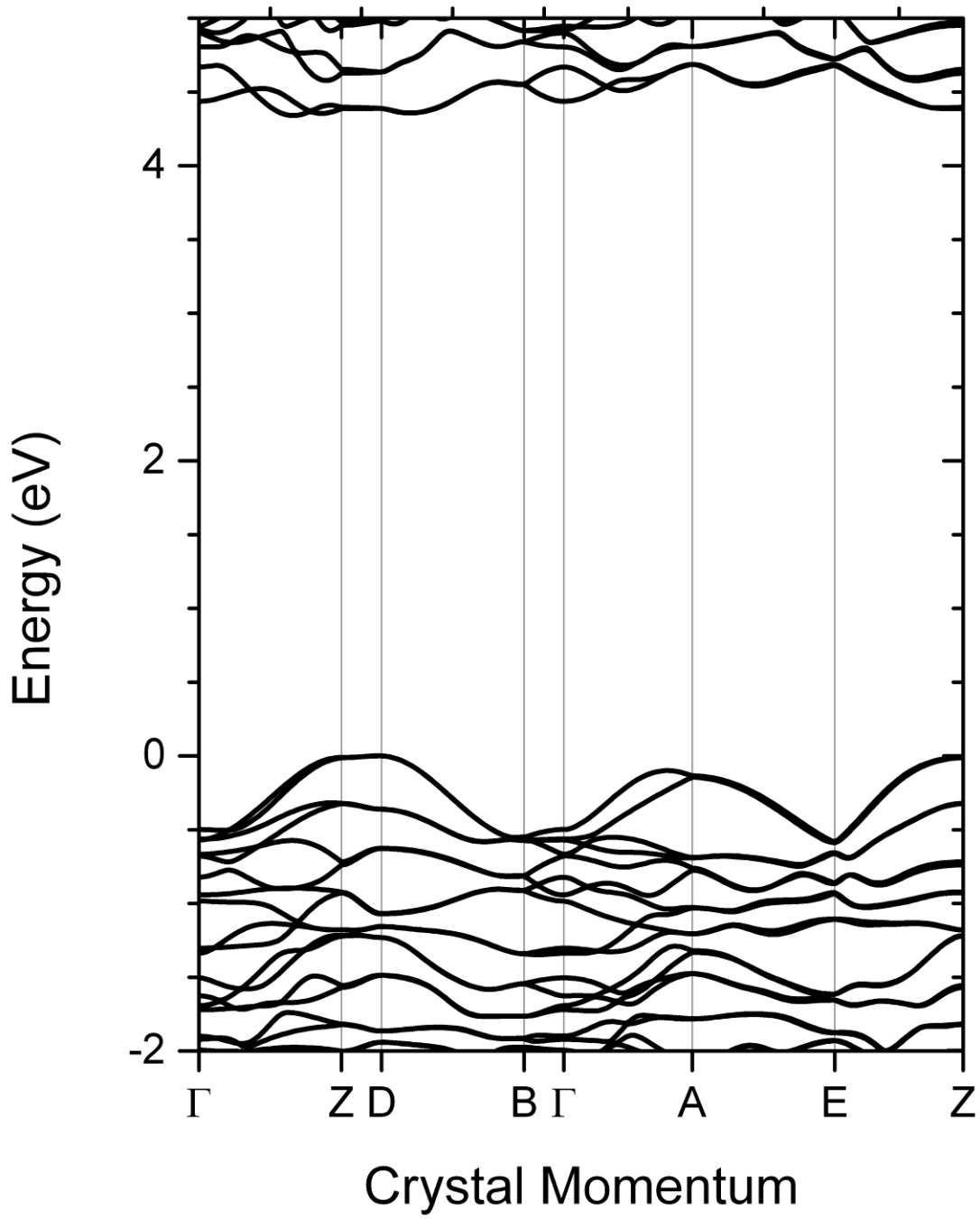

Figure S2. Near band-edge calculated band structure of BP_3N_6. The horizontal axis of the band structure panel corresponds to a path through high symmetry points in the Brillouin zone.

Table S1. Formation energies of nitrogen vacancies in BP_3N_6. Nitrogen vacancies were added to each crystallographically unique nitrogen site of a $2 \times 2 \times 1$ supercell of BP_3N_6.

Defect	N_{1v}	N_{2v}	N_{3v}	N_{4v}	N_{5v}	N_{6v}
Formation Energy (eV)	4.53	4.51	4.46	4.23	2.49	2.89

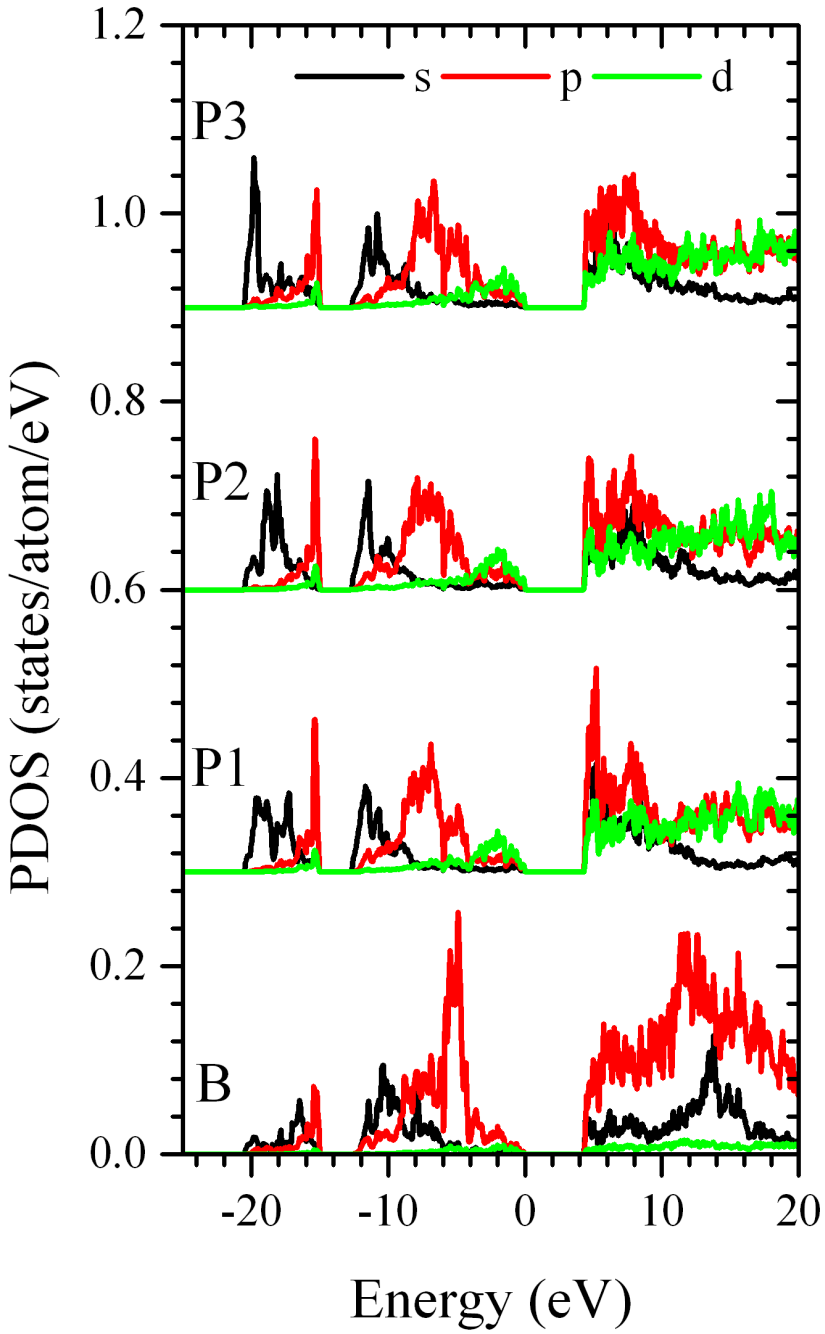

Figure S3. Calculated partial density of states (PDOS) of the B and P atoms of BP_3N_6, with the atoms as labelled with the PDOS vertically offset for clarity. The calculation was performed with the PBEsol exchange-correlation functional.

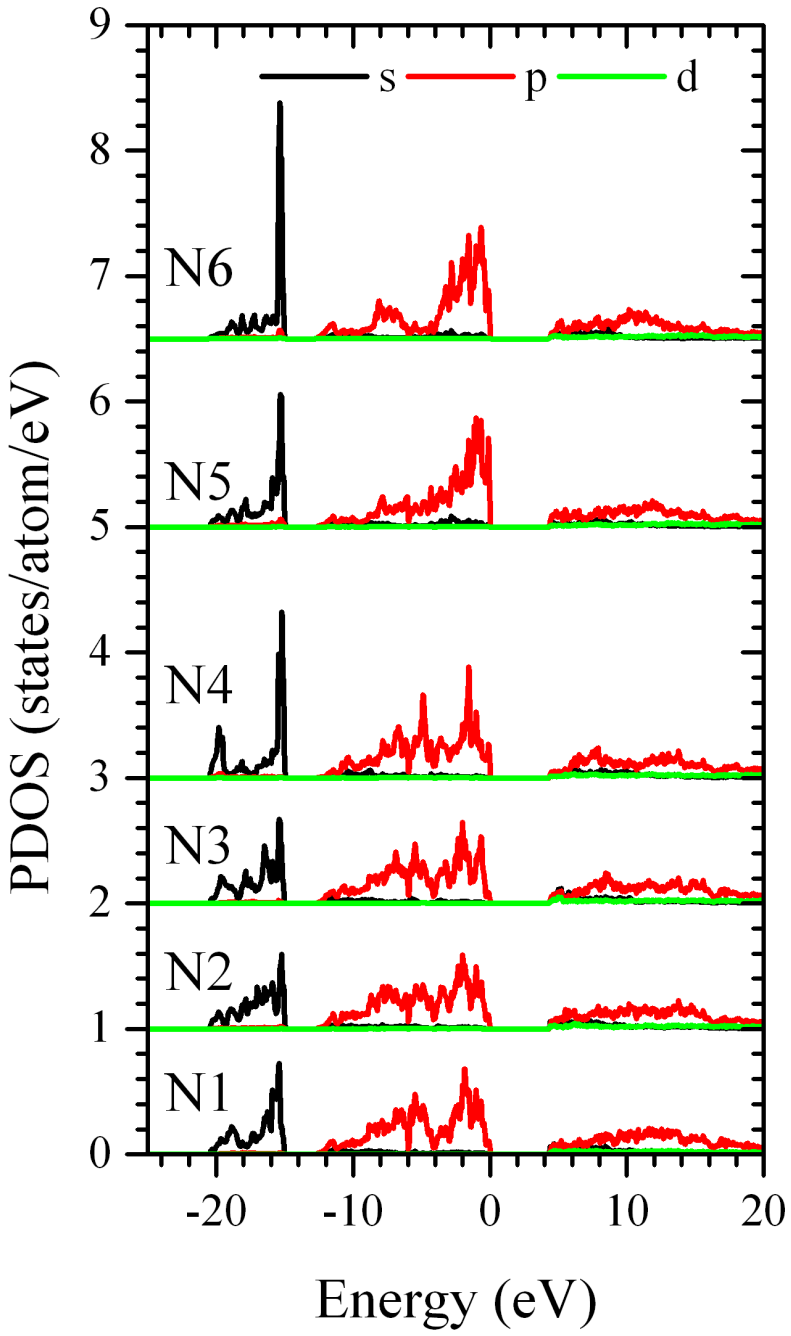

Figure S4. Calculated partial density of states (PDOS) of the N atoms of BP_3N_6, with the atoms as labelled with the PDOS vertically offset for clarity. The calculation was performed with the PBEsol exchange-correlation functional.