On the low-energy phases of bismuthene

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Abstract

We employ an ab-initio structure search algorithm to explore the configurational space of Bi in quasi two dimensions [1]. A confinement potential restricts the movement of atoms within a pre-defined thickness during structure search calculations within the minima hopping method to find the stable and metastable forms of bilayer Bi. In addition to recovering the two known low-energy structures (puckered monoclinic and buckled hexagonal), our calculations predict three new structures of bi-layer Bi. We call these structures the α, β, and γ phases of bilayer Bi, which are, respectively, 63, 72, and 83meV/atom higher in energy than the monoclinic ground state, and thus potentially synthesizable using appropriate substrates. We also compare the structural, electronic, and vibrational properties of the different phases. The puckered monoclinic, buckled hexagonal, and β phases exhibit a semiconducting energy gap, whereas α and γ phases are metallic. We notice an unusual Mexican-hat type band dispersion leading to a van Hove singularity in the buckled hexagonal bilayer Bi. Notably, we find symmetry-protected topological Dirac points in the electronic spectrum of the γ phase. The new structures suggest that bilayer Bi provides a novel playground to study distortion-mediated metal-insulator phase transitions.

References

[1] S. Singh et al., arXiv:1901.05060 (2019).

Figures

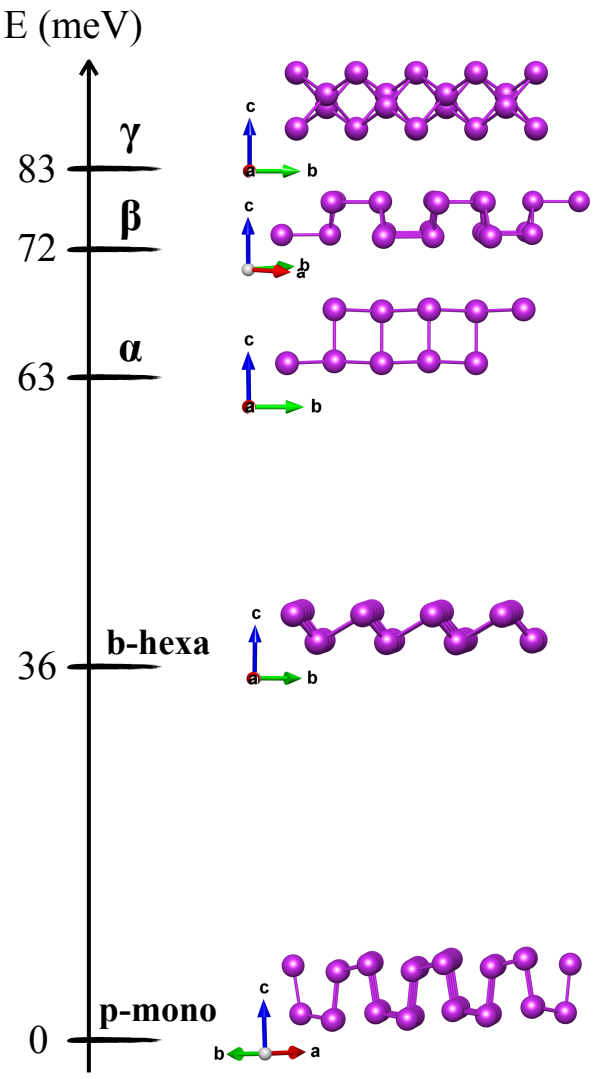

Figure 1: Energetic ordering and relaxed structures of the low-energy phases of bilayer Bi (side view). The energy differences between the structures (in meV/atoms) are reported with respect to the formation energy of the puckered monoclinic (p-mono) structure.