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Pentaoctite Phase of Group-V Nanostructures

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Abstract

Recently, the existence of an allotrope phase of bismuthene called pentaoctite, in which all hexagonal rings are replaced by either pentagons or octagons, has been proposed.[1,2] These structures show a sizeable bandgap, can be stable under strain, and have topological insulator behavior with protected surface nontrivial Dirac states. From this information, we extend our investigations of this allotrope phase to phosphorene,[3]arsenene,[4,5] and antimonene.[6,7] Our first-principles calculations show that these 2D structures are metastable against their respective hexagonal phases, but have relatively low formation energies. In particular, group-V pentaoctite can become a direct gap material under tensile or compressive strain. Our calculated dielectric function shows that all structures have absorption edges in the visible region, making these materials suitable for optoelectronic applications.

References

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