

Electronic and Optical Properties of newly Predicted, Metallic Penta-Bipyramidal Boron

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Bulk orthorhombic boron (o-B₁₄) is a recently predicted, three-dimensional boron allotrope which has fascinating properties[1]. Its structure is characterized by edge-sharing pentagonal bipyramids with diverse bond lengths ranging from 1.644 to 1.966 Å as shown in the Figure below. These structural motifs facilitate the formation of unusual seven-centre-two-electron π -bonds, which are identified for the first time in three-dimensional boron allotropes. The presence of these bonds highlights the complexity and versatility of boron chemistry under ambient conditions. Moreover, this material is predicted to be a superconductor with a T_c value of 29.1 K.

The present work employs the first-principles calculations based on the GGA-PBE functional to explore the atomic and electronic properties of o-B₁₄. The result would provide insight into the electronic band structure, density of states, and bonding characteristics. Moreover, we further investigate the optical and plasma dispersion properties of o-B₁₄. These calculations would reveal distinctive anisotropic behaviors, broadening its potential applications in plasmonics and beyond.

The calculation of bandstructure exhibits its metallic behavior with three bands crossing the Fermi level. These bands consist of steep bands and flat bands near the Fermi level. The steep bands promote high electron velocities, while the flat bands enhance the density of states and favor electronic interactions.

Such electronic features suggest the potential for unique transport and quantum properties. Furthermore, within the structural units, we observed a strong orbital hybridization between the B 2p orbitals. It reinforces the stability of the bonding framework. The anticipated plasmonic and optical responses, driven by the anisotropic bonding network, offer promising opportunities for advanced optoelectronic and quantum devices.

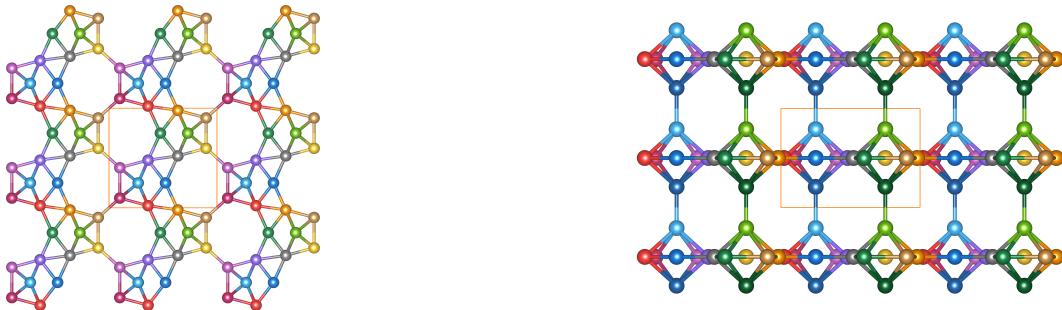


Figure 1: Top view (left) and side view (right) of o-B₁₄ pentagonal bipyramidal bulk.

References

- [1] S. Han, Y. Liu, C. Wang, W. Yi, X. Chen, Y. Zhang, and X. Liu, *Superconducting boron allotrope featuring pentagonal bipyramid at ambient pressure*, Phys. Chem. Chem. Phys., **25**, 15400 (2023).