Unveiling New Horizons in 2D Materials: Computational Discovery of a Metallic Boron Nitride Monolayer

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The hexagonal boron nitride (hBN) monolayer, sharing the same crystalline structure and isoelectronic properties with graphene, is well-recognized for its wide band gap semiconductor nature (~6 eV) attributed to the predominantly ionic BN bonds. Addressing the diverse requirements of applications has driven the exploration for stable boron nitride configurations featuring considerably reduced band gaps, particularly those with metallic characteristics. Herein, using density functional theory (DFT) computations and inspired by our discovery of the highly aromatic (BNN)6 molecular structure, which can serve as building blocks, we theoretically designed a novel two-dimensional (2D) boron nitride material that exhibits metallic behavior driven by the intriguing phenomenon of electron conjugation. Our computations showed that this new BN monolayer is kinetically stable and has decent thermodynamic, mechanic, and thermal stabilities, indicating its high feasibility for experimental realization. This work unveils a hitherto unexplored 2D BN material distinguished by its unique geometric configuration, metallic attributes, and the high likelihood of successful experimental production. It is another example to vividly demonstrate the importance of chemical concepts in rational materials design, and further extensions likely result in other novel 2D materials with exceptional properties.

Awards Won:
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