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Computational design of three-dimensional metallic boron nitride[1] QIAN WANG, SHUNHONG ZHANG, Center for Applied Physics and Technology, Peking University, YOSHIYUKI KAWAZOE, Institute for Material Research, Tohoku University, Japan, PURU JENA, Virginia Commonwealth University, Virgina, USA, PEKING UNIVERSITY TEAM, TOHOKU UNIVERSITY COLLABORATION, VIRGINIA COMMONWEALTH UNIVERSITY COLLABORATION — Based on comprehensive calculations, we have shown that the 3D BN structures composed of interlocking BN hexagons are metallic and dynamically stable. These newly designed 3D BN structures (T-BxNx, x=4n-1, n=1, 2, 3...) are hybrid systems with one B and one N atom in sp3 hybridization and (4n-2) sp2-bonded B and N atoms respectively per unit cell. The sp3 bonded B (N) atom binds to its surrounding four sp2 bonded N (B) atoms forming the 3D backbone and is responsible for stability. The sp2 bonded B atoms, on the other hand, play the key role in rendering the conducting network and metallicity. This special geometrical feature results in a unique property: unlike previously reported functionalized c-BN thin film whose metallicity stems from strong inbuilt polarization, the metallicity in 3D T-BxNx is intrinsic and comes from the delocalized electrons distributed around the B sites. The metallicity exhibited in the studied structures opens new door for BN materials with potential applications in electron transport, metal-free catalysis and electronic devices.

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