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A new structure of two-dimensional allotropes of group V elements PING LI, WEIDONG LUO, Shanghai Jiao Tong University — The elemental two-dimensional (2D) materials such as graphene, silicene, germanene, and black phosphorus have attracted considerable attention due to their fascinating physical properties. Structurally they possess the honeycomb or distorted honeycomb lattices, which are composed of six-atom rings. Here we find a new structure of 2D allotropes of group V elements composed of eight-atom rings, which we name as the octagonal tiling (OT) structure. First-principles calculations indicate that these allotropes are dynamically stable and are also thermally stable at temperatures up to 600 K. These allotropes are semiconductors with band gaps ranging from 0.3 to 2.0 eV, thus they are potentially useful in near- and mid-infrared optoelectronic devices. OT-Bi is also a 2D topological insulator (TI) with a band gap of 0.33 eV, which is the largest among the reported elemental 2D TIs, and this gap can be increased further by applying compressive strains.

Ping Li
Shanghai Jiao Tong University

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