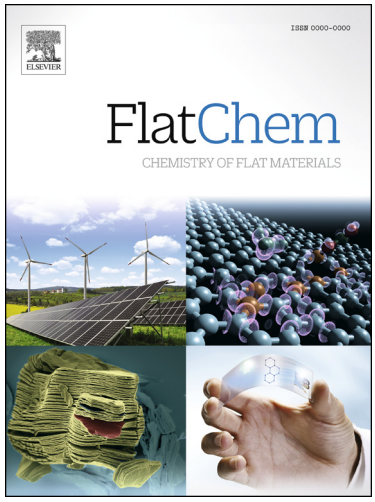

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MnB_x Monolayers with Quasi-Planar Hypercoordinate Mn Atoms and Unique Magnetic and Mechanical Properties

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Abstract

Searching and designing two-dimensional (2D) materials with unique topological structures and physical and chemical properties is extremely significant in the field of materials science. Here we report the design of 2D MnB_x (x = 1, 2, 3, 6) monolayers containing quasi-planar hypercoordinate motifs by means of density functional theory (DFT) computations and particle swarm optimization technique. These systems exhibit high cohesive energy as well as good kinetic and thermal stability, indicating that the MnB_x monolayers can be prepared in experiments. Bond order analyses suggest that the abundance of multicenter bonds contributes to the stability of MnB_x monolayers. Among them, MnB_3 monolayer has nonmagnetic ground state while others exhibit ferromagnetic metallic properties. Moreover, MnB_6 monolayer exhibits high spin polarization and negative Poisson's ratio, which endows MnB_6 with many special applications to cushioning and nanoelectronics.

Keywords: MnB_x monolayers, ferromagnetic, metallic, auxeticity