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Crystal structure and phase stability of tungsten borides[1] QUAN LI, DAN ZHOU, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA, YANMING MA, State Key Laboratory of Superhard Materials, Jilin University, Changchun 130012, China, CHANGFENG CHEN, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA — We address the longstanding and controversial issue of ground-state structures of technically important tungsten borides using a first-principles structural search method via a particle-swarm optimization (PSO) algorithm. We have explored a large set of stable chemical compositions (convex hull) and clarified the ground-state structures for a wide range of boron concentrations, including W_2B, W_3B_2, WB, W_2B_3, WB_2, W_2B_5, WB_3, and WB_4. We further assessed relative stability of various tungsten borides and compared the calculated results with previously reported experimental data. The phase diagram predicted by the presented calculations may serve as a useful guide for synthesis of a variety of tungsten borides.

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