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Stabilization of Small Boron Cage by Transition Metal Encapsulation[1] LIJUN ZHANG, JIAN LV, YANCHAO WANG, YANMING MA, Jilin University, China — The discovery of chemically stable fullerene-like structures formed by elements other than carbon has been long-standing desired. On this aspect significant efforts have centered around boron, only one electron deficient compared with carbon. However, during the past decade a large number of experimental and theoretical studies have established that small boron clusters are either planar/quasi-planar or forming double-ring tubular structures. Until recently, two all-boron fullerenes have been independently discovered: B_{38} proposed by our structure searching calculations[1] and B_{40} observed in a joint experimental and theoretical study. Here we extend our work to the even smaller boron clusters and propose an effective routine to stabilize them by transition metal encapsulation. By combining swarm-intelligence structure searching and first-principles calculations, we have systematically investigated the energy landscapes of transition-metal-doped MB_{24} clusters (M = Ti, Zr, Hf, Cr, Mo, W, Fe, Ru and Os). Two stable symmetric endohedral boron cages, MoB_{24} and WB_{24} are identified. The stability of them can be rationalized in terms of their unique 18-electron closed-shell electronic structures.
[1] J. Lv, Y. Wang, L. Zhu, and Y. Ma, Nanoscale 6, 11692 (2014).

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