

**Supporting Information for**  
**Structural and Electronic Properties of Single-atom Transition**  
**Metal-doped Boron Clusters MB<sub>24</sub> (M=Sc, V, Mn)**

Yue-Ju Yang, Shi-Xiong Li,\* De-Liang Chen, Zheng-Wen Long

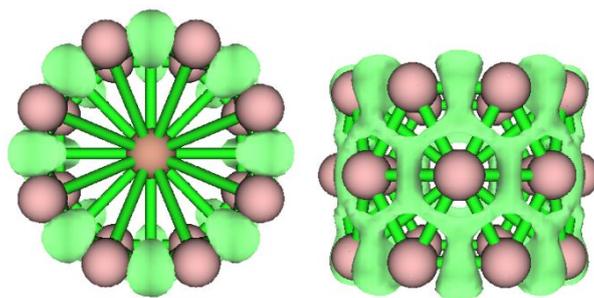
**Yue-Ju Yang** — School of Physics and Electronic Science, Guizhou Education University, Guiyang 550018, P.R.China

**Shi-Xiong Li** — School of Physics and Electronic Science, Guizhou Education University, Guiyang 550018, P.R.China

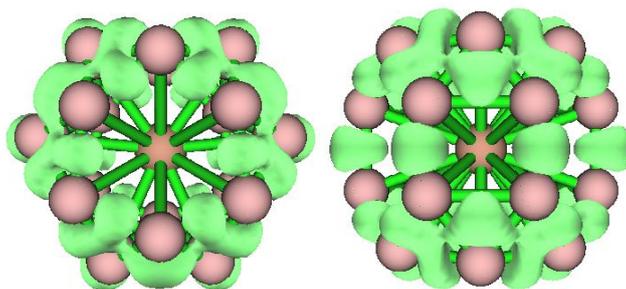
**De-Liang Chen** — School of Physics and Electronic Science, Guizhou Education University, Guiyang 550018, P.R.China

**Zheng-Wen Long** — College of physics, Guizhou University, Guiyang 550025, P.R.China

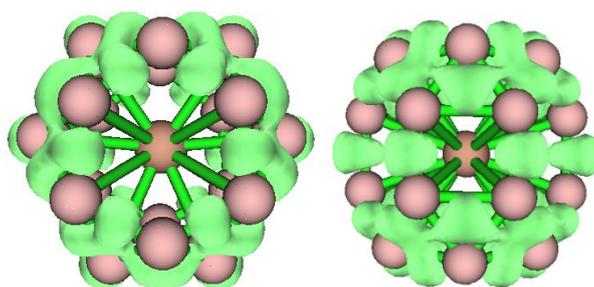
\*email: [leesxoptics@163.com](mailto:leesxoptics@163.com)



(a)

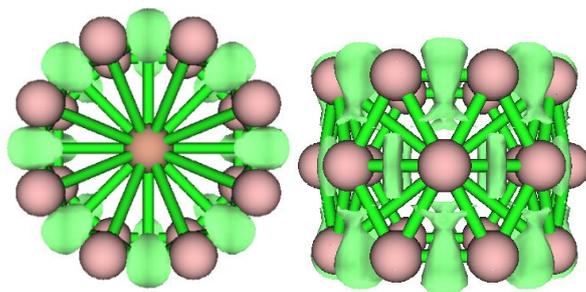


(b)

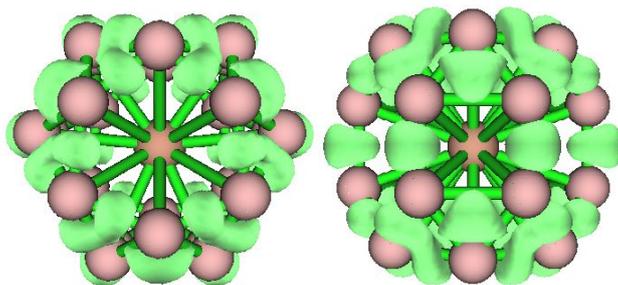


(c)

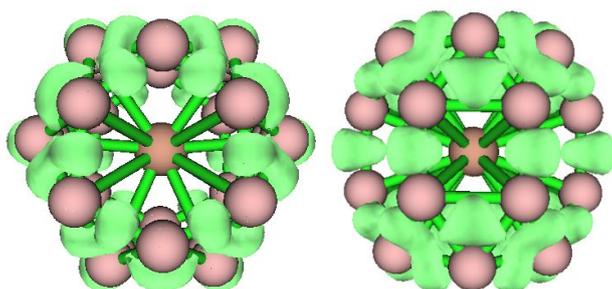
**Figure S1.** LOL with the isovalue set to 0.72. The left is top view and right is side view. (a) ScB<sub>24</sub>; (b) VB<sub>24</sub>; (c) MnB<sub>24</sub>.



(a)

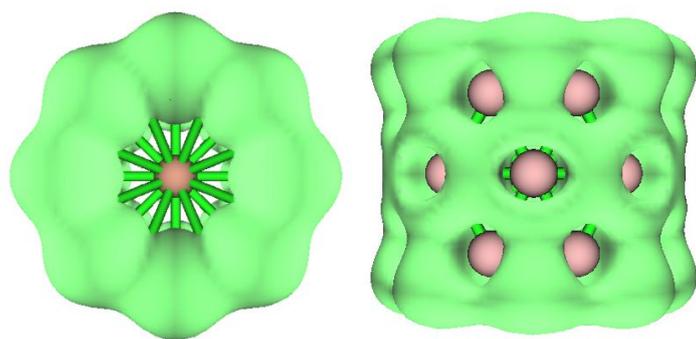


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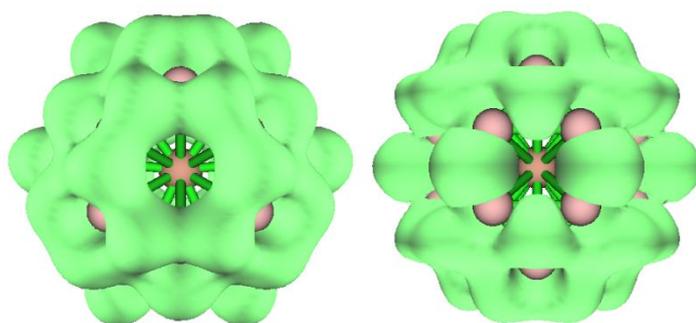


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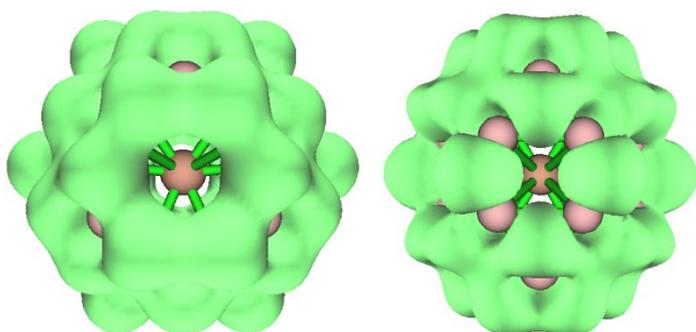
**Figure S2.** LOL with the isovalue set to 0.73. The left is top view and right is side view. (a) ScB<sub>24</sub>; (b) VB<sub>24</sub>; (c) MnB<sub>24</sub>.



(a)

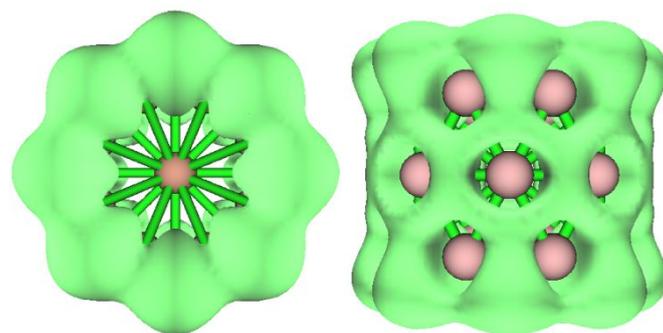


(b)

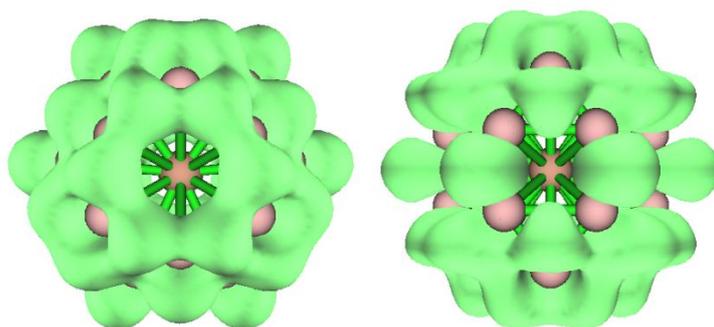


(c)

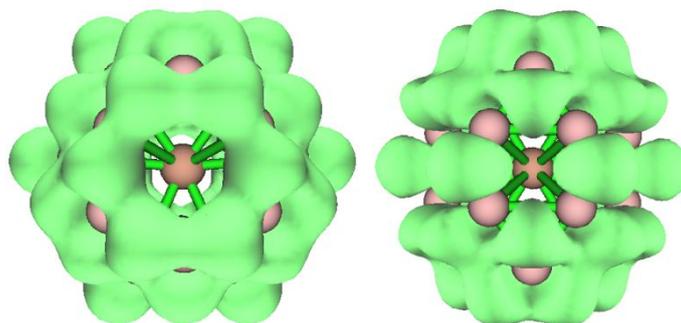
**Figure S3.** Electron localization function (ELF) with the isovalue set to 0.80. The left is top view and right is side view. (a)  $\text{ScB}_{24}$ ; (b)  $\text{VB}_{24}$ ; (c)  $\text{MnB}_{24}$ .



(a)

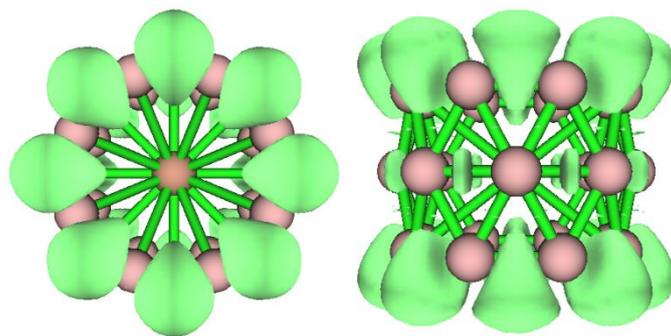


(b)

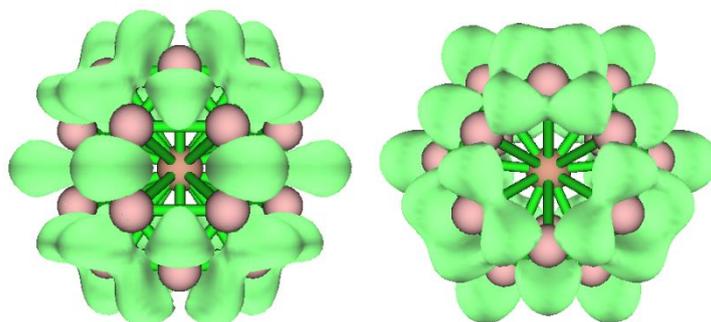


(c)

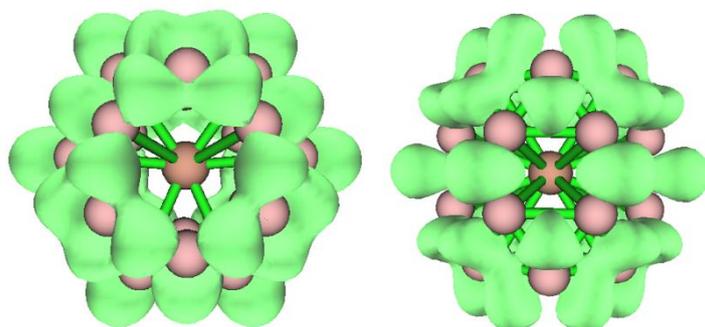
**Figure S4.** Electron localization function (ELF) with the isovalue set to 0.84. The left is top view and right is side view. (a)  $\text{ScB}_{24}$ ; (b)  $\text{VB}_{24}$ ; (c)  $\text{MnB}_{24}$ .



(a)

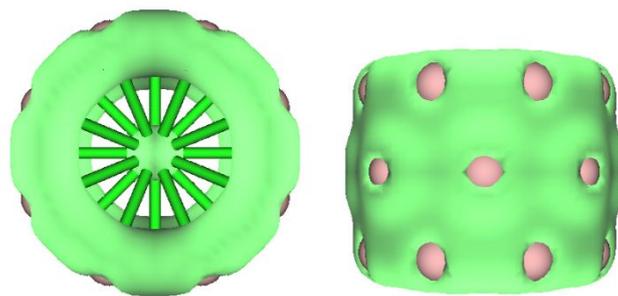


(b)

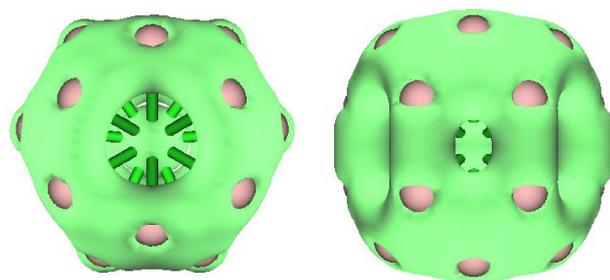


(c)

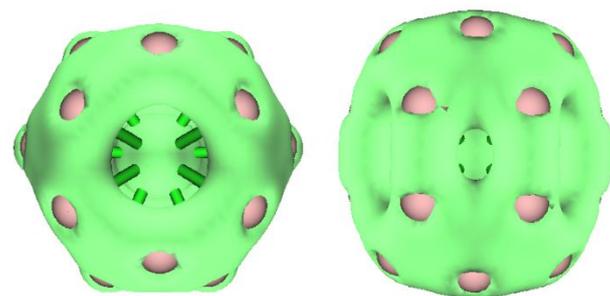
**Figure S5.** Electron localization function (ELF) with the isovalue set to 0.89. The left is top view and right is side view. (a) ScB<sub>24</sub>; (b) VB<sub>24</sub>; (c) MnB<sub>24</sub>.



(a)

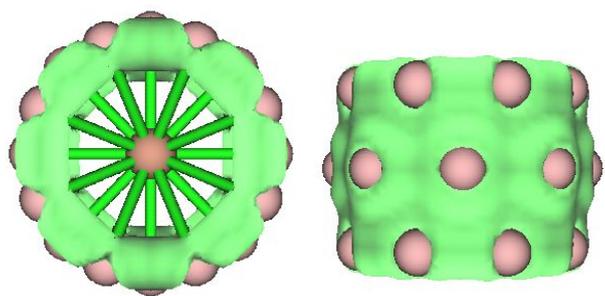


(b)

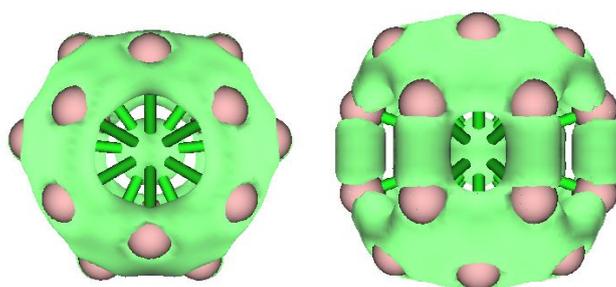


(c)

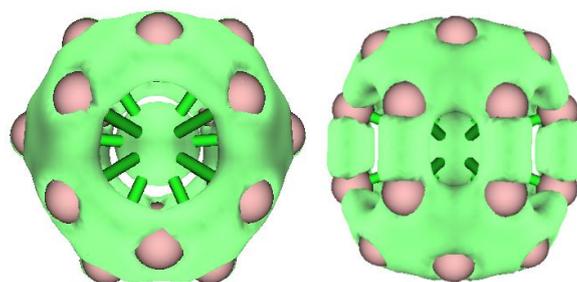
**Figure S6.** Valence electron density with the isovalue set to 0.16. The left is top view and right is side view. (a) ScB<sub>24</sub>; (b) VB<sub>24</sub>; (c) MnB<sub>24</sub>.



(a)

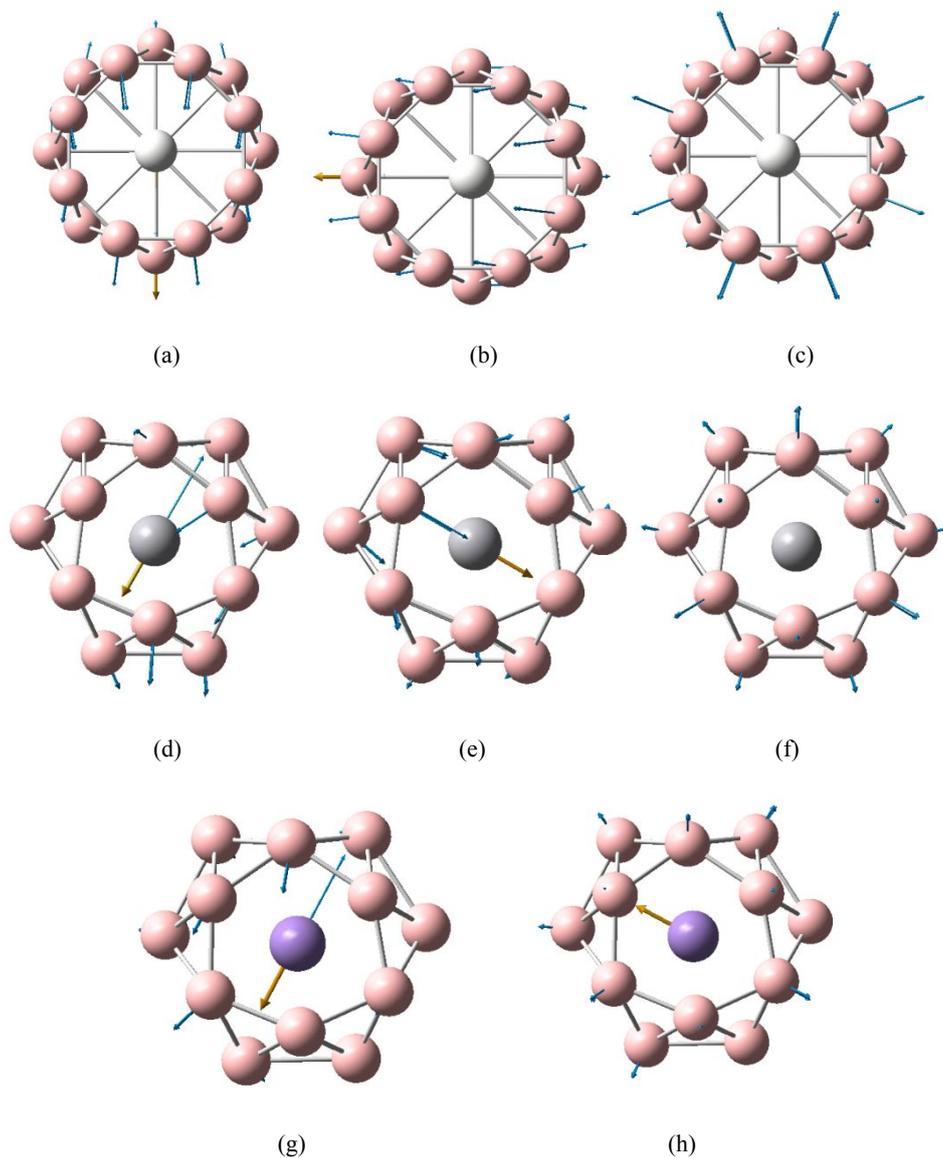


(b)



(c)

**Figure S7.** Valence electron density with the isovalue set to 0.20. The left is top view and right is side view. (a)  $\text{ScB}_{24}$ ; (b)  $\text{VB}_{24}$ ; (c)  $\text{MnB}_{24}$ .



**Figure S8.** Vibrational modes. (a) and (b) the degenerate strongest infrared-active modes of  $\text{ScB}_{24}$ , (c) the strongest Raman-active mode of  $\text{ScB}_{24}$ , (d) and (e) the degenerate strongest infrared-active modes of  $\text{VB}_{24}$ , (f) the strongest Raman-active mode of  $\text{VB}_{24}$ , (g) the strongest infrared-active mode of  $\text{MnB}_{24}$ , and (h) the strongest Raman-active mode of  $\text{MnB}_{24}$ .