

Tunable Dirac states in doping B₂S₃ monolayer

Xiaoteng Li,^{*†1} Xi Zuo,^{†2} Bin Cui,³ Wenkai Zhao,¹ Yuqing Xu,¹ Dongqing Zou,¹ Chuanlu Yang^{*1}

To discuss the rationality of the doped B₂S₃ monolayers, we calculate their formation energies (ΔE)¹ as shown in Table R1. ΔE is defined as $\Delta E = E(M_xB_yS_z) - xE(M) - yE(B) - zE(S)$, ($M = C, N, Sn$). It is clear that the difference between the pristine B₂S₃ and the M-doped B₂S₃ is pretty small, about 0.041, 0.049, and 0.039 eV, respectively. It indicates that it is reasonable for these doped configurations.

Table S1 The formation energies of B₂S₃, C/N/Sn-doped B₂S₃.

Materials	Formation energy (eV/Å ²)
B ₂ S ₃	-0.076
C-doped B ₂ S ₃	-0.035
N-doped B ₂ S ₃	-0.027
Sn-doped B ₂ S ₃	-0.037

References

1. X. Li, X. Zuo, H. Li, L. Han, Q. Gao, D. Li, B. Cui, D. Liu and F. Qu, *Physical chemistry chemical physics: PCCP*, 2019, **21**, 19234-19241.

¹ School of Physics and Optoelectronic Engineering, Ludong University, Yantai 264000, People's Republic of China

² College of Physics and Electronic Science, Hubei Normal University, Huangshi 435002, China

³ School of Physics, State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100, People's Republic of China

[†] These authors contributed equally to this work.