

## Supplementary Information

### **First-principles study on electronic states of $\text{In}_2\text{Se}_3/\text{Au}$ heterostructure controlled by strain engineering**

Sha Han, Cai-Juan Xia\*, Min Li, Xu-Mei Zhao, Guo-Qing Zhang, Lian-Bi Li, Yao-

Heng Su, Qing-Long Fang\*

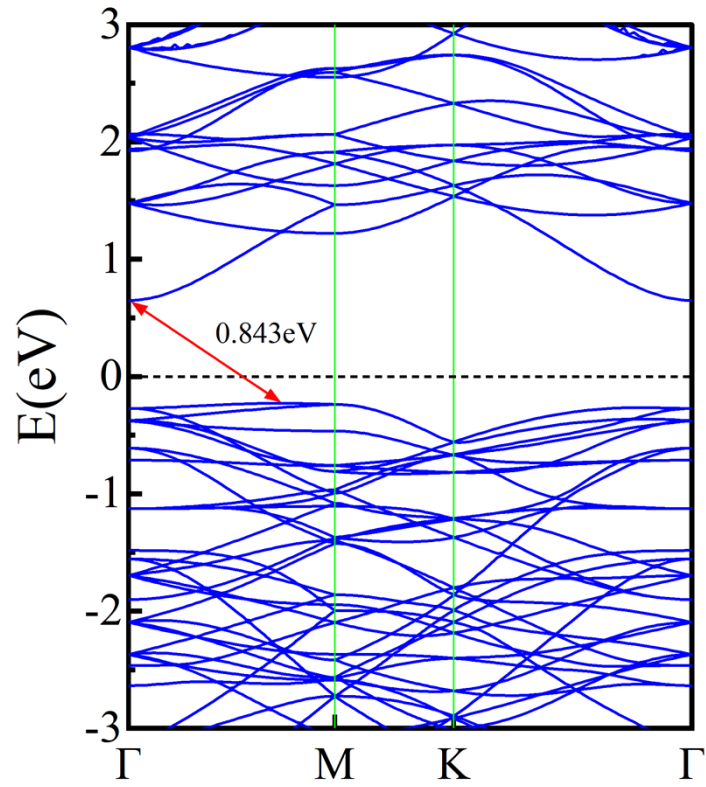
*School of Science, Xi'an Polytechnic University, Xi'an 710048, Shaanxi, China  
Engineering Research Center of Flexible Radiation Protection Technology,  
University of Shaanxi Province, Xi'an Polytechnic University, Xi'an 710048, Shaanxi,  
China*

*Xi'an Key Laboratory of Nuclear Protection Textile Equipment Technology, Xi'an  
Polytechnic University, Xi'an 710048, Shaanxi, China*

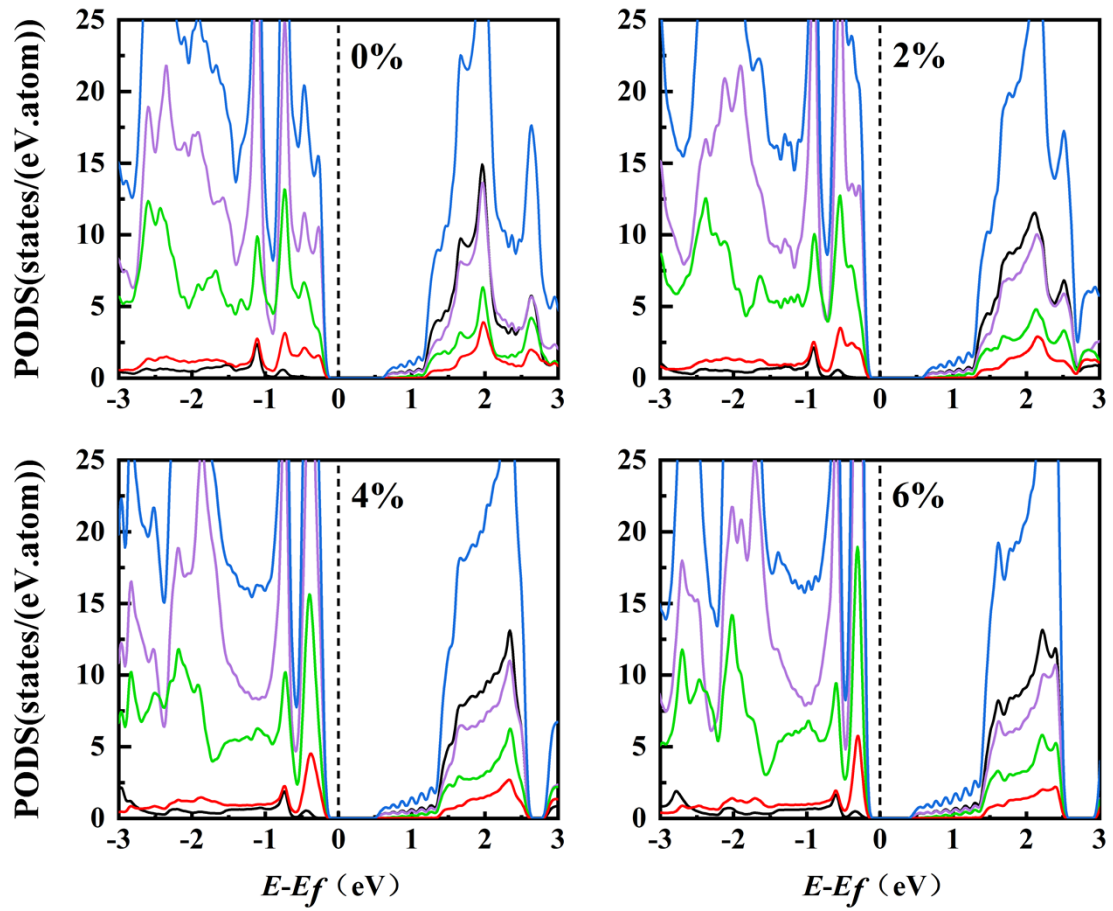
\* Corresponding authors.

E-mail addresses: [caijunxia@xpu.edu.cn](mailto:caijunxia@xpu.edu.cn) (Cai-Juan Xia);

[qinglong\\_fang@xpu.edu.cn](mailto:qinglong_fang@xpu.edu.cn) (Qing-Long Fang).



**Figure. S1.** Band structure of monolayer  $\text{In}_2\text{Se}_3$ . The Fermi level is set to zero energy and is denoted by the dashed line.



**Figure. S2.** Partial density of states (PDOS) of  $\text{In}_2\text{Se}_3$  under biaxial tensile strain. The black, purple, green, red and blue lines represent the In s, In p, Se s, Se p and the total density of states, respectively. The black vertical dashed line represents Fermi level.