

## Supporting Information

### **DFT Study of Zn-Modified SnP<sub>3</sub>: A H<sub>2</sub>S Gas Sensor with Superior Sensitivity, Selectivity, and Fast Recovery Time**

Hongyuan Cui<sup>a,b</sup>, Chenshan Gao<sup>c</sup>, Pengwei Wang<sup>a,b</sup>, Lijie Li<sup>d</sup>, Huaiyu Ye<sup>c</sup>, Zhongquan Wen<sup>a</sup>, Yufei Liu<sup>a,b,d,\*</sup>

<sup>a</sup> Key Laboratory of Optoelectronic Technology & Systems (Chongqing University), Ministry of Education, Chongqing 400044, China

<sup>b</sup> Centre for Intelligent Sensing Technology, College of Optoelectronic Engineering, Chongqing University, Chongqing 400044, China

<sup>c</sup> School of Microelectronics, Southern University of Science and Technology, Shenzhen 518055, China

<sup>d</sup> Faculty of Science and Engineering, Swansea University, Swansea SA1 8EN, UK

\*To whom correspondence should be addressed

Key Laboratory of Optoelectronic Technology & Systems (Chongqing University),

Ministry of Education, Chongqing 400044, China

E-mail address: Yufei.Liu@cqu.edu.cn

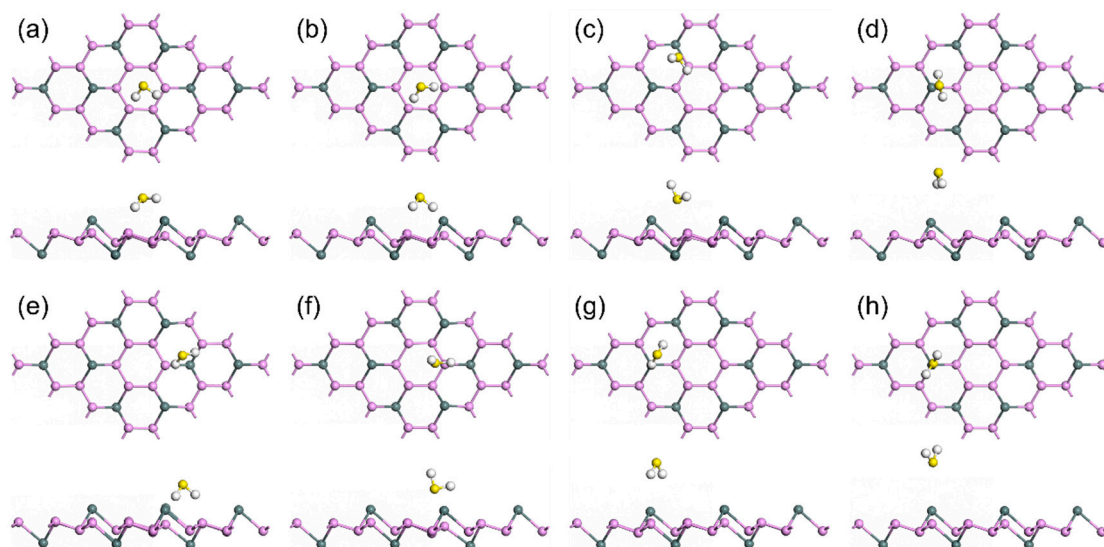


Fig. S1. Multiple optimized structures of intrinsic SnP<sub>3</sub> monolayer for H<sub>2</sub>S adsorption.

(a) H<sub>2</sub>S is horizontally adsorbed on the P atom (P-H).

(b) H<sub>2</sub>S is horizontally adsorbed on the P atom (P-S).

(c) H<sub>2</sub>S is horizontally adsorbed on the Sn atom (Sn-H).

(d) H<sub>2</sub>S is horizontally adsorbed on the Sn atom (Sn-S).

(e) H<sub>2</sub>S is vertically adsorbed on the P atom (P-H).

(f) H<sub>2</sub>S is vertically adsorbed on the P atom (P-S).

(g) H<sub>2</sub>S is vertically adsorbed on the Sn atom (Sn-H).

(h) H<sub>2</sub>S is vertically adsorbed on the Sn atom (Sn-S).

Atom color code: H–white, S–yellow, Sn–grey, and P–purple.

Fig. S1 shows a variety of optimized structures of intrinsic SnP<sub>3</sub> after H<sub>2</sub>S adsorption. Horizontal adsorption is the placement of the H<sub>2</sub>S molecule horizontally above the SnP<sub>3</sub> monolayer and is divided into two cases: H-atom alignment and S-atom alignment. Vertical adsorption is the placement of the H<sub>2</sub>S molecule vertically above the SnP<sub>3</sub> monolayer and is divided into two cases: H-atom alignment and S-atom alignment.

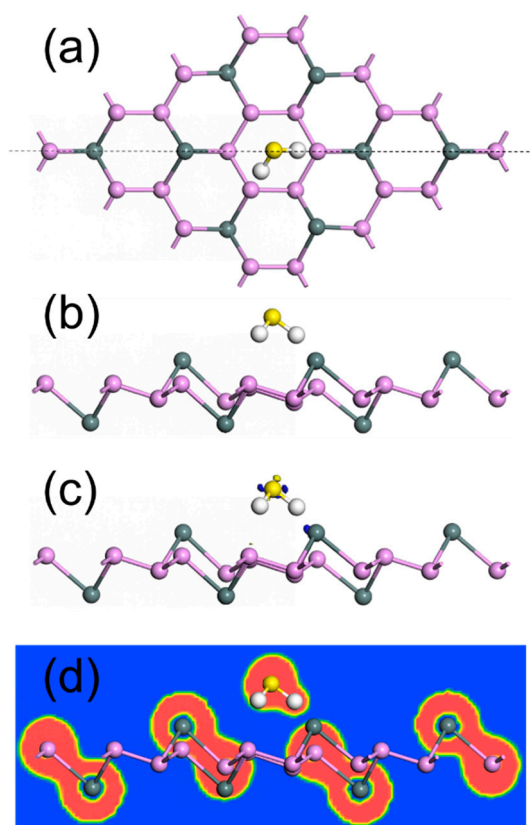


Fig. S2. (a)-(b) Top and side views of the most stable structure of intrinsic SnP<sub>3</sub> monolayer adsorbed H<sub>2</sub>S, (c) charge density difference (CDD), (d) electron localization function (ELF).

Fig. S2(a) and S2(b) show the top and side views of the most stable structure of the intrinsic SnP<sub>3</sub> monolayer adsorbed H<sub>2</sub>S (as in the case of Fig. S1(b)). Fig. S2(c) and S2(d) show the CDD and ELF, respectively.

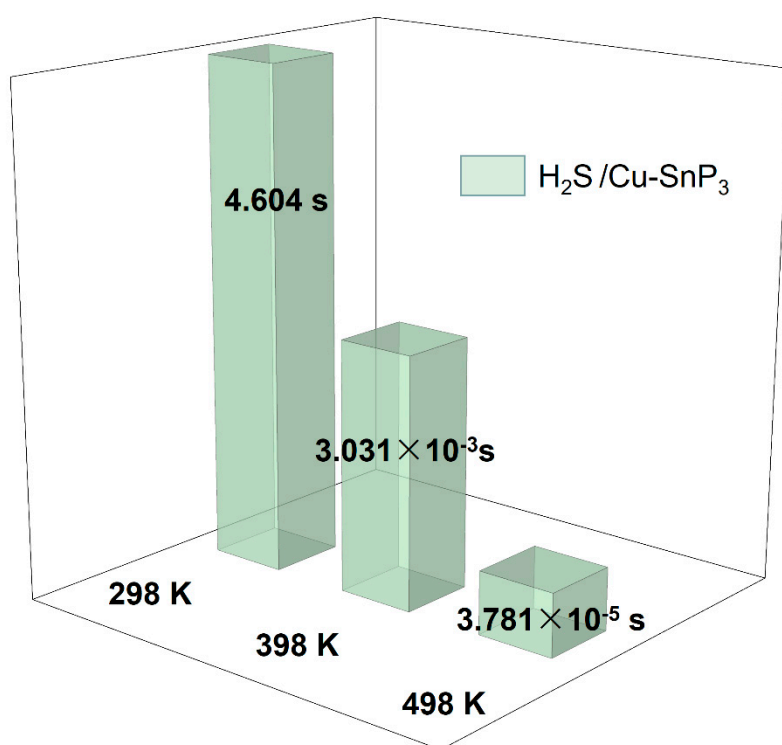


Fig. S3. The recovery time of H<sub>2</sub>S adsorbed on Cu-SnP<sub>3</sub> at 298 K, 398 K, and 498 K, respectively.