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Electronic Supplementary Information for Novel two-dimensional semiconductor SnP_3: high stability, tunable bandgaps and high carrier mobility explored by first-principles calculations

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INTERLAYER INTERACTION IN THE SNP_3 MLTILAYER

In order to understand the intrinsic mechanism for the change from metal to semiconductor, two aspects needs to be considered. Firstly, the structure of SnP_3, can be described as a layer structure related to the As-type structure in which the corrugated layers are composed of puckered P_6rings as shown in Fig. 1. The layers thus formed are stacked upon one another perpendicular to the c axis so that a distorted octahedral environment of P atoms is formed around each of the Sn atoms, which results in significant puckering and a pseudo-Jahn-Teller distortion. We calculated the interlayer interaction from the multilayer to bilayer and the results (Figure. S1) illustrate that the interlayer interaction for SnP_3 systems decreases from tetralayer to bilayer. Thus, we believe that the dependence of the interlayer interaction on the layer thickness most likely plays an important role in the metal to semiconductor transition in the SnP_3 layered systems. Meanwhile, the quantum confinement effect may be another factor that affects the electronic structure transition. When the multilayer with metallic character reduced to semiconductive bilayer, the conduction bands shift towards the vacuum level.

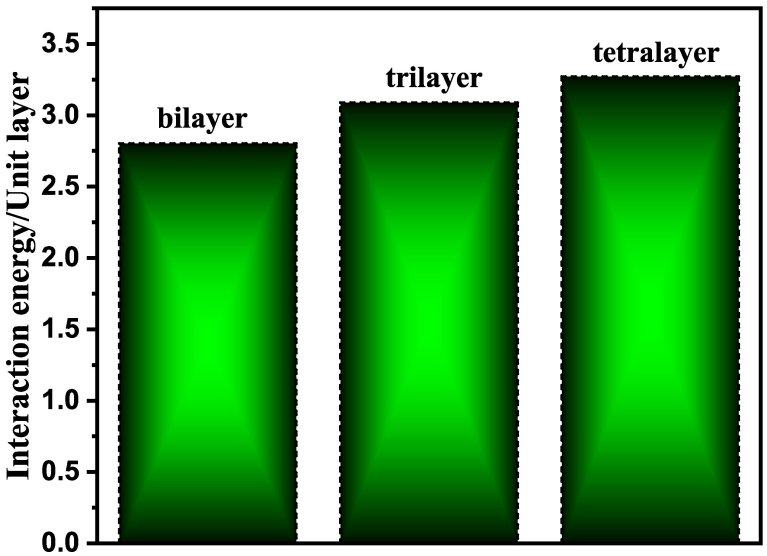

Figure S1. Interlayer interaction energies (eV) of SnP_3 bilayer, trilayer, tetralayer.

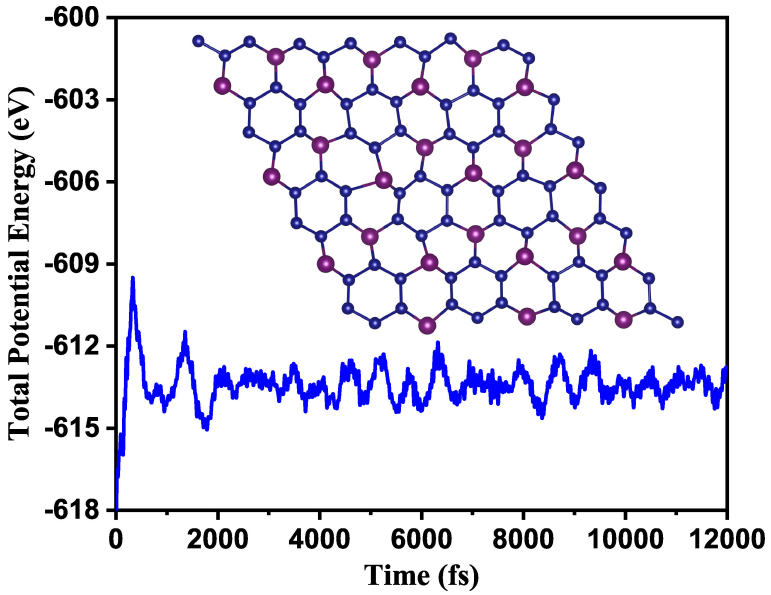

Figure S2. Total potential energy of SnP_3 monolayer during AIMD simulations at 300 K. The inset shows the snapshot at the end of simulation.

THERMAL STABILITY

The thermal stability of SnP_3 monolayer is examined by performing AIMD simulations in the canonical ensemble. After evolving for 12 picoseconds (ps) at room temperature (300K) with a time step of 1 femtoseconds (fs), no structural reconstruction was observed at the end of the simulation (12 ps). The total potential energy is stabilized at around 2 ps, as shown in Fig. S2. The results suggest that the SnP3 monolayer is thermally stable.

THE RESPONSE OF MECHANICAL PROPERTIES OF SNP_3 MONOLAYER AND BILAYER TO THE ELASTIC STRAIN

When the applied strains are in the elastic range, the strain energy $\triangle E$ has quadratic dependence on the value of applied strains ε (the strain energy is defined as the difference between the total energy of the system with strain $E(\varepsilon)$ and that without strain $E(0)$). Following the method based on first-principles calculations described in the previous work,[1, 2] we have investigated several strained structures and calculated the total energy of the corresponding fully relaxed structures, and found that the applied strains on SnP_3 monolayer (bilayer) in our manuscript, which are in the range from -6% to 12% (-7% to 7%), are in

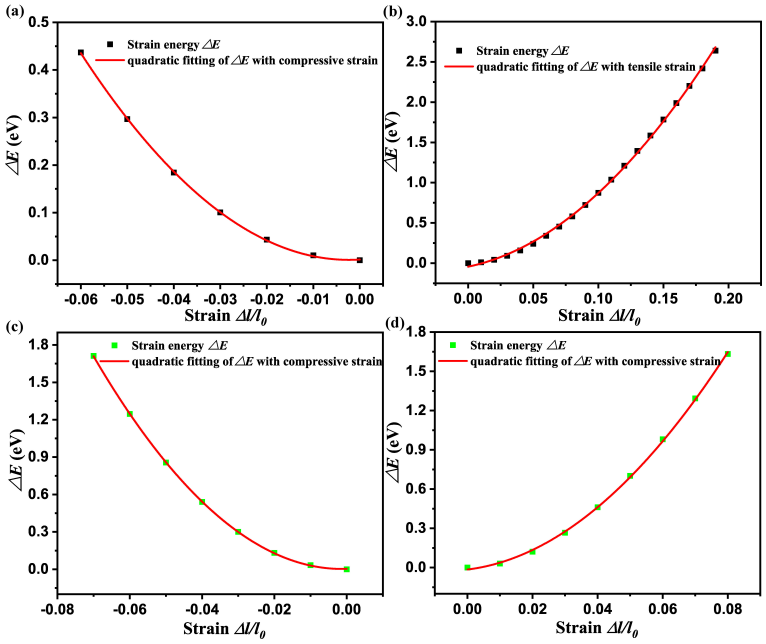

Figure S3. The relation of the strain energy $\triangle E$ and the biaxial strain for SnP_3 monolayer (a), (b) and bilayer (c), (d), respectively.

the corresponding elastic range, as shown in Fig. S3.

[1] H. Şahin, S. Cahangirov, M. Topsakal, E. Bekaroglu, E. Akturk, R. T. Senger, and S. Ciraci, Physical Review B **80**, 155453 (2009).

[2] R. Qin, C.-H. Wang, W. Zhu, and Y. Zhang, Aip Advances **2**, 022159 (2012).