Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

Mechanical and transport properties of $InGeX_3$ (X=S, Se and Te) monolayer using density functional theory and machine learning

Yong-Bo Shi,[1] Yuan-Yuan Chen,[1] Hao Wang,[1] Shuo Cao,[2] Heng-Xu Zhu,[3] Meng-Fan Chu,[4] Zhu-Feng Shao,[1] Hai-Kuan Dong,[1,*] and Ping Qian[3,†]

[1] *College of Physical Science and Technology, Bohai University, Jinzhou 121013, PR China*
[2] *Beijing Advanced Innovation Center for Materials Genome Engineering, Corrosion and Protection Center, University of Science and Technology Beijing, Beijing 100083, PR China*
[3] *Department of Physics, University of Science and Technology Beijing, Beijing 100083, PR China*
[4] *College of Miami, Henan University, Kaifeng 475004, PR China*

* donghaikuan@163.com
† qianping@ustb.edu.cn

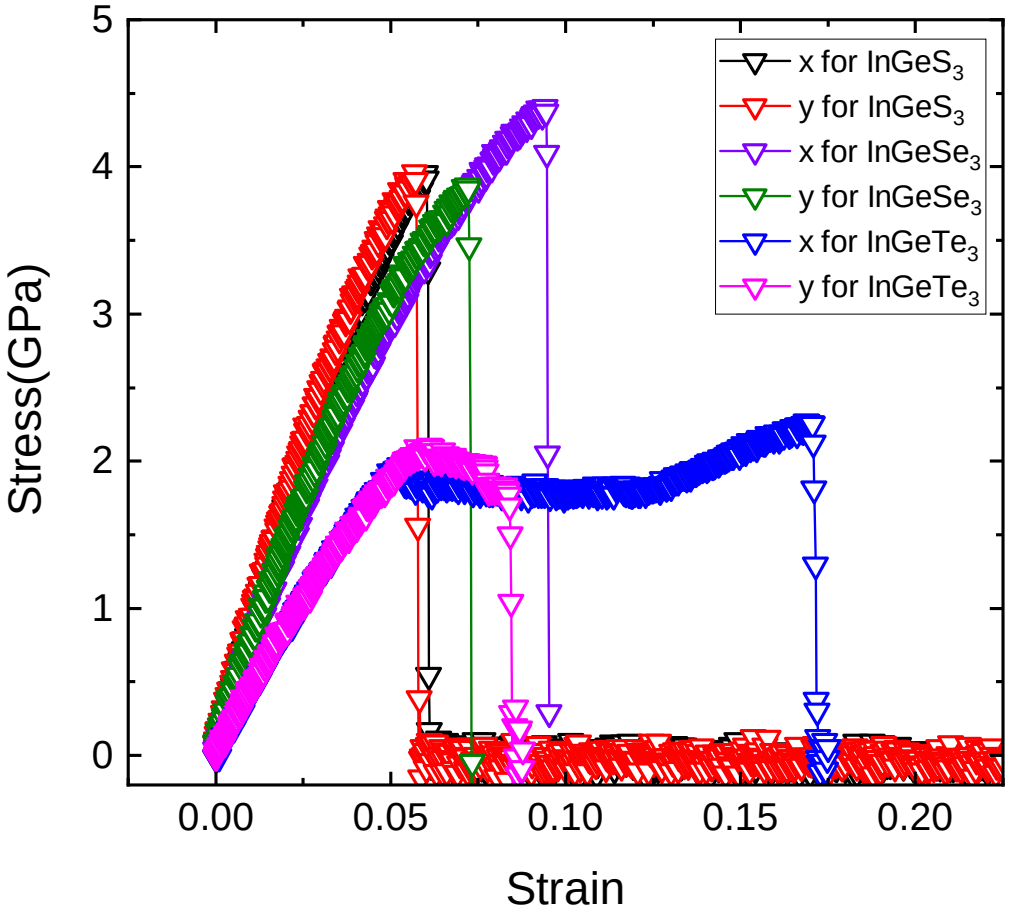

Figure S1. Stress as a function of uniaxial strain for $InGeX_3$ (X=S, Se and Te) monolayer calculated by NEP-based MD simulations at 300 K.

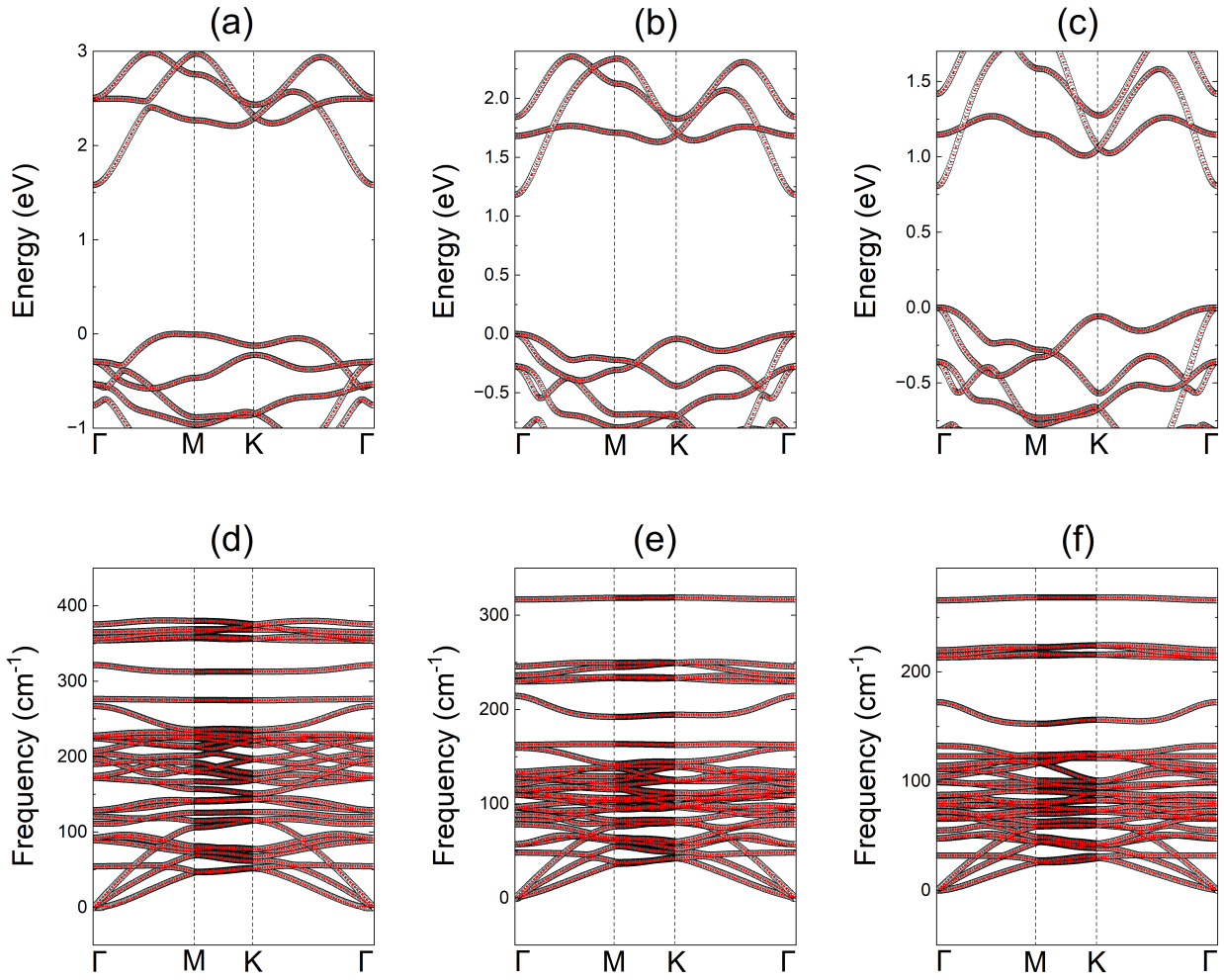

Figure S2. The electronic band structure of $InGeX_3$ (X=S, Se and Te) monolayer calculated from DFT (symbol in black) and Wannier interpolation approach (symbol in red)