# Supplemental Materials for

# Theoretical Prediction of stress-tunable Optoelectronic Properties of GaSeI: A Novel 1D Helical van der Waals Crystals

Zhuo Zhao[1,2], Jian Zhang[2,3], Feng Xiao[4,5], Baotian Wang[5], Yee Sin Ang[6*], Daxin Liang[1*], Gang Zhang[2,3*]

[1] Key Laboratory of Bio-based Material Science & Technology (Ministry of Education), Northeast Forestry University, Harbin 150040, China

[2] Yangtze Delta Region Academy of Beijing Institute of Technology (Jiaxing), Jiaxing 314019, China

[3] School of Materials Science and Engineering, Beijing Institute of Technology, Beijing 100081, China

[4] School of Physics, Sun Yat-Sen University, Guangzhou 510275, China

[5] Institute of High Energy Physics, Chinese Academy of Science, Beijing 100049, China

[6] Science, Mathematics and Technology, Singapore University of Technology and Design, Singapore 487372, Singapore

Corresponding author. E-mail: yeesin_ang@sutd.edu.sg; daxin.liang@nefu.edu.cn; zhanggang@bitjx.edu.cn

## 1. Figures.

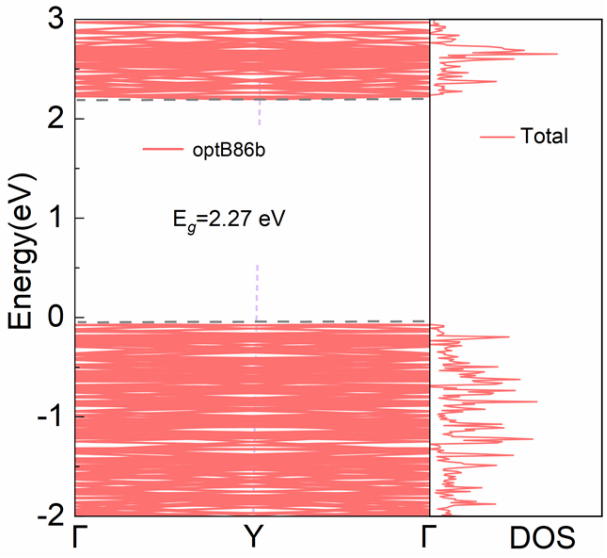


Figure S1. The calculated electronic band structures of GaSeI nanochain with the inclusion of SOC.

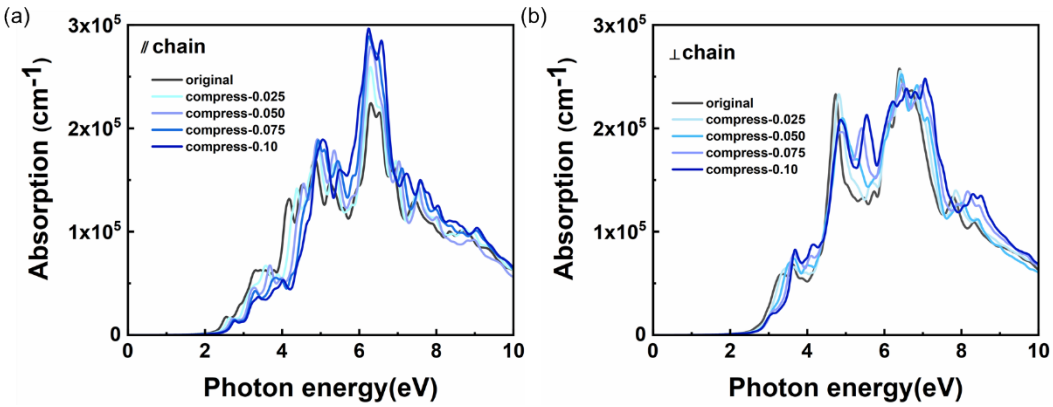


Figure S2. (a, b) The absorption coefficients of 1D GaSeI under compress stress along the chain and perpendicular to the chain directions, respectively.

**2. The carrier mobility.**

The effective mass $m^*$ is defined as $m^* = \hbar^2\left(\frac{\partial^2 E}{\partial k^2}\right)^{-1}$ , and $C^{1D}$ is the stretching modulus defined as $C^{1D} = \frac{1}{c_0}\frac{\partial^2 E}{\partial \varepsilon^2}$ ,where $E$ is the total energy, $\varepsilon$ is the applied strain, and $c_0$ is the lattice constant of the 1D system in equilibrium. $E_1$ is the DP constant of VBM for holes or that of CBM for electrons, $c_0$ as defined by $E_1 = \left|\frac{dE_{edge}}{d\varepsilon}\right|$ ,where $E_{edge}$ is the energy of the conduction (or valence) band edge.