

Electronic Supplementary Information

Strain-engineering the electronic properties and anisotropy of GeSe₂ monolayer

Zong-Bao Li,^a Xia Wang,^a Wei Shi,^a Xiao-bo Xing^b, Ding-Jiang Xue^{*c}, and Jin-Song Hu^c

^aSchool of Material and Chemical Engineering, Tongren University, Tongren 554300, China

^bMOE Key Laboratory of Laser Life Science & Institute of Laser Life Science, College of Biophotonics, South China Normal University, Guangzhou 510631, China

^cCAS Key Laboratory of Molecular Nanostructure and Nanotechnology, Beijing National Research Center for Molecular Sciences, CAS Research/Education Center for Excellence in Molecule Science, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China

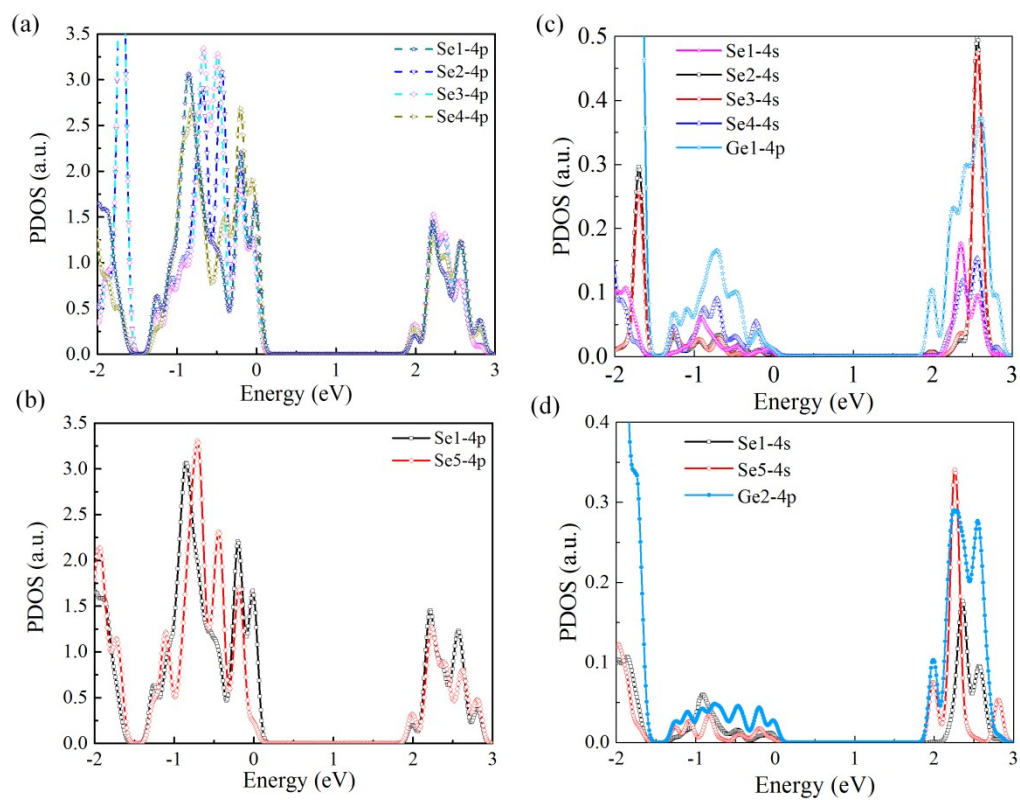


Fig. S1 PDOSs of different atoms in GeSe_2

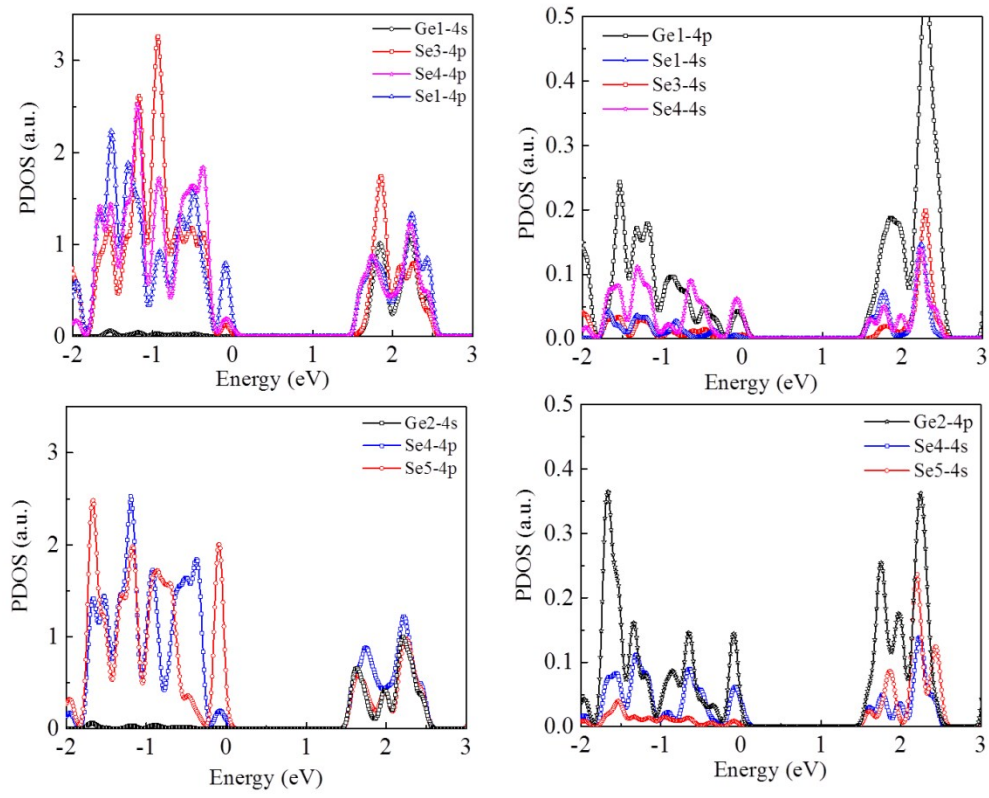


Fig. S2 PDOSs of the main atoms states under strain $\varepsilon_y = -12\%$

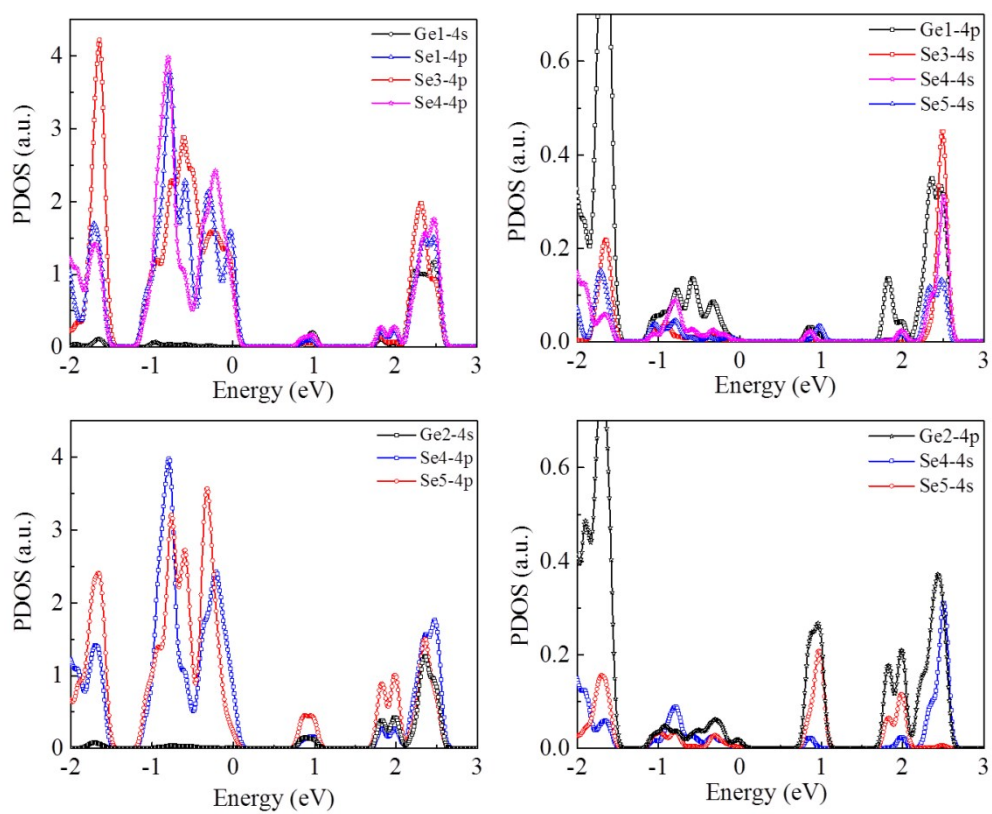


Fig. S3 PDOSs of the main atoms states under strain $\epsilon_y = 12\%$

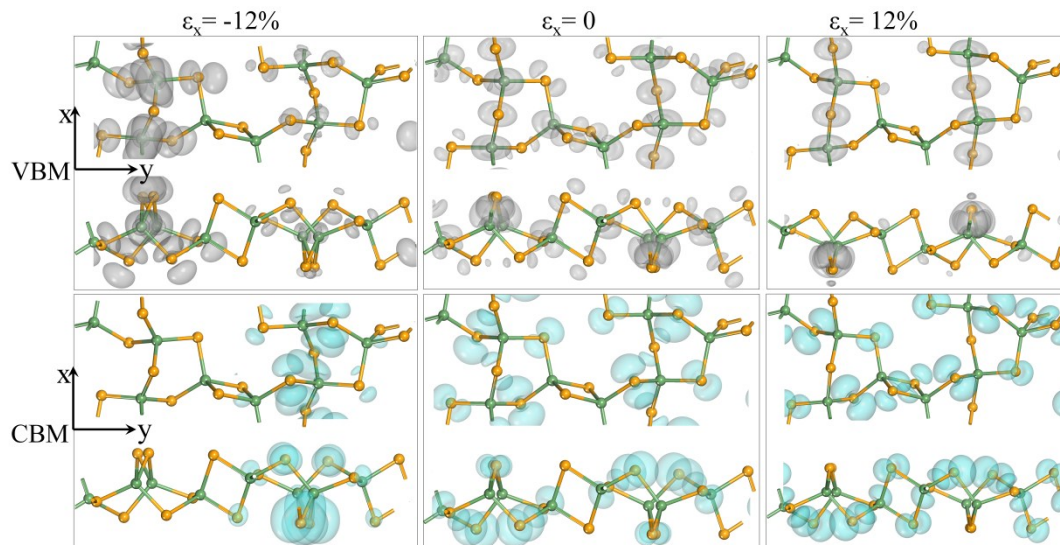


Fig. S4 The charge density contour plots of the VBM and CBM in GeSe₂ monolayer under different strains of $\epsilon_x=12\%$ and $\epsilon_x=-12\%$. The isovalue is same.