

# Supporting Information for

## Janus Layers and Electronic Structure of 1T-(TiSeS)<sub>2</sub>

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# Table of Contents

1. Fig S1: Crystal structures of  $(\text{TiSeS})_2$ -186 — S3
2. Fig S2: Atom-resolved phonon dispersions of the 1T-TiS<sub>2</sub> — S3
3. Fig S3: Atom-resolved phonon dispersions of the 1T-TiSe<sub>2</sub> — S4
4. Fig S4: Atom-resolved phonon dispersions of the 1T- $(\text{TiSeS})_2$  — S4
5. Fig S5: Atom-resolved phonon dispersions of the TiSeS-156 — S5
6. Fig S6: Atom-resolved phonon dispersions of the  $(\text{TiSeS})_2$ -186 — S5
7. Fig S7: Phonon dispersions of 1T- $(\text{TiSeS})_2$ , TiSeS-156, and  $(\text{TiSeS})_2$ -186 — S6
8. Fig S8: PBE+vdW-DF band structures — S6
9. Fig S9: PBE0+vdW-DF band structures — S7
10. Fig S10: PBE+vdW-DF, DFT+U, and PBE0+vdW-DF band structures for  $(\text{TiSeS})_2$ -186 — S7
11. Fig S11: Optical conductivity  $\sigma_{ii}(\omega)$  of 1T- $(\text{TiSeS})_2$ , TiSeS-156, and  $(\text{TiSeS})_2$ -186 — S8

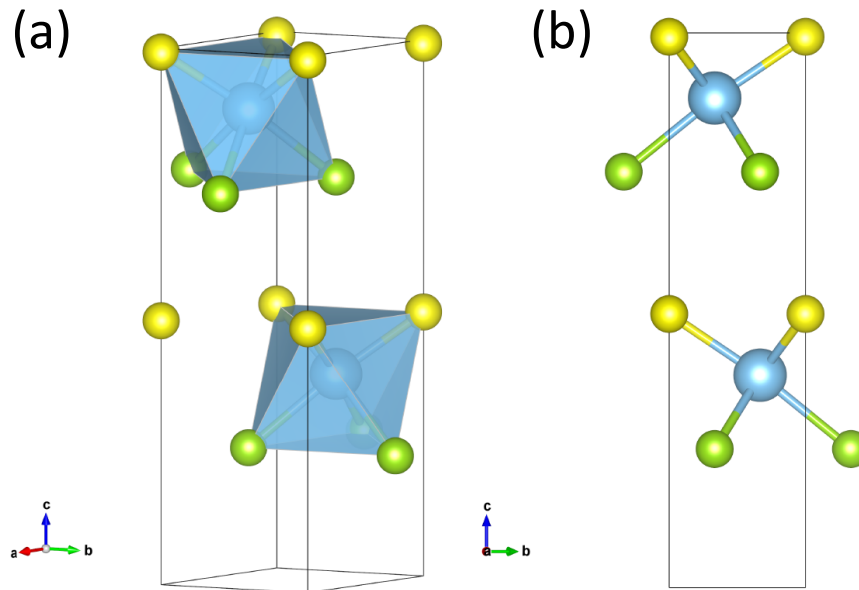


Figure S1: (color online) Crystal structures of  $(\text{TiSeS})_2\text{-186}$ . The black lines denote the unit cells. The graphical representation was prepared using VESTA3.

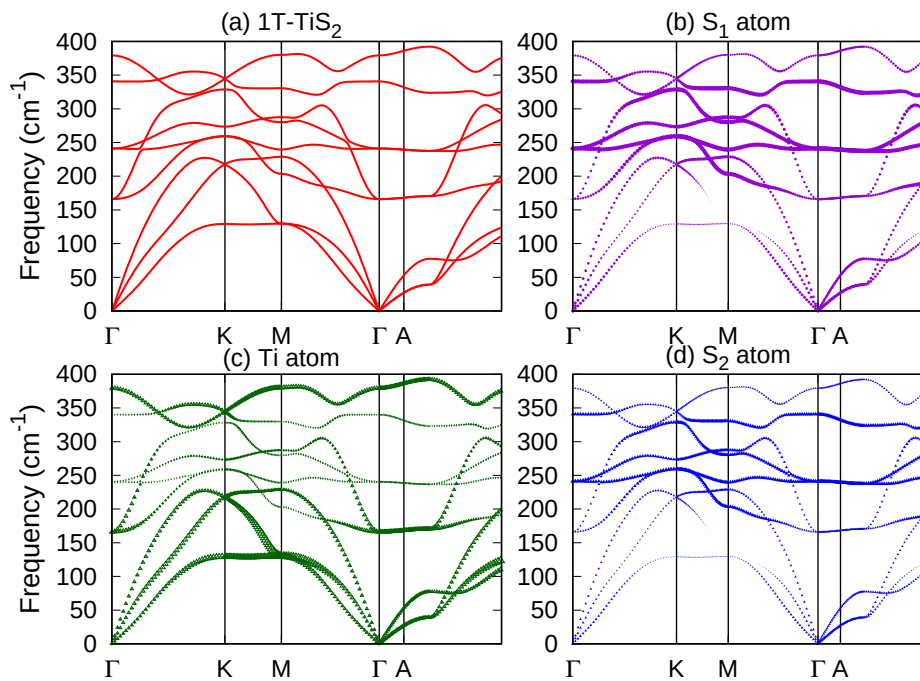


Figure S2: (color online) Atom-resolved phonon dispersions of the 1T-TiS<sub>2</sub>. Contribution of atom-resolved phonon dispersion, (a) All atoms, (b) S<sub>1</sub> atom, (c) Ti atom, and (d) S<sub>2</sub> atom.

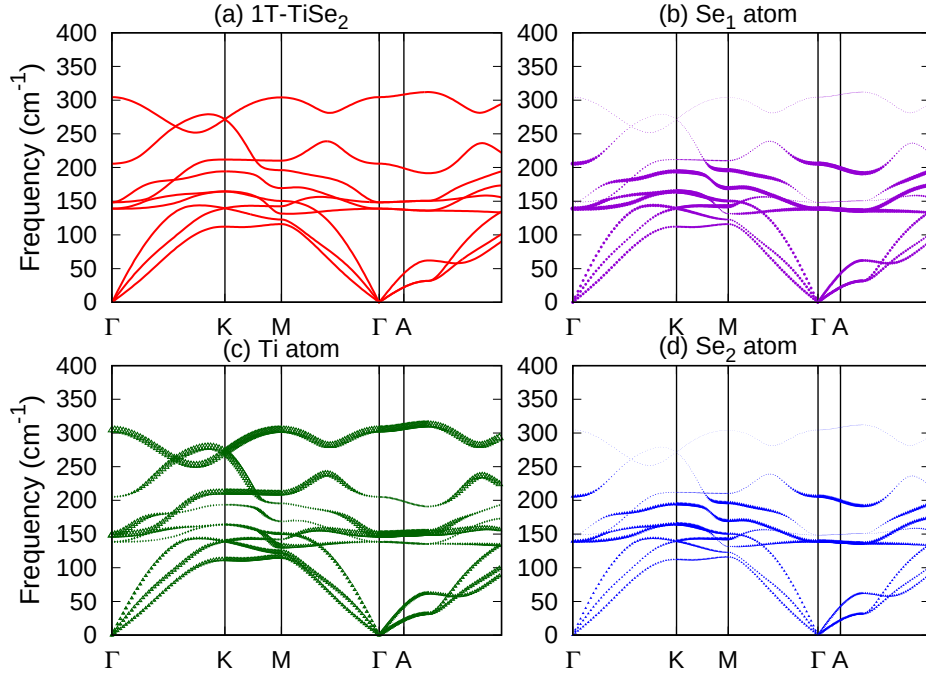


Figure S3: (color online) Atom-resolved phonon dispersions of the 1T-TiSe<sub>2</sub>. Contribution of atom-resolved phonon dispersion, (a) All atoms, (b) Se<sub>1</sub> atom, (c) Ti atom, and (d) Se<sub>2</sub> atom.

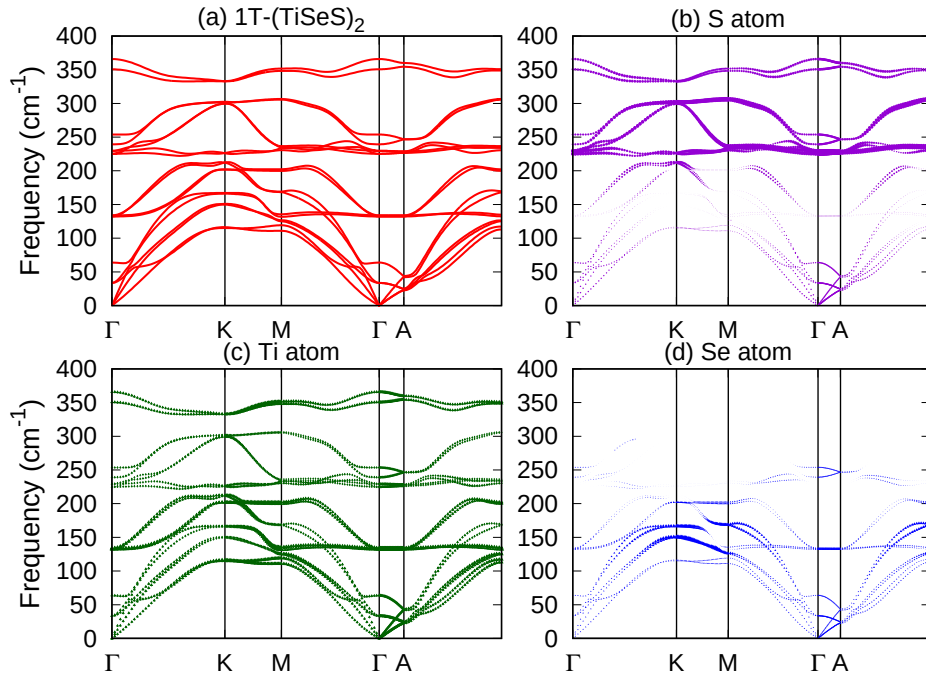


Figure S4: (color online) Atom-resolved phonon dispersions of the 1T-(TiSeS)<sub>2</sub>. Contribution of atom-resolved phonon dispersion, (a) All atoms, (b) S atom, (c) Ti atom, and (d) Se atom.

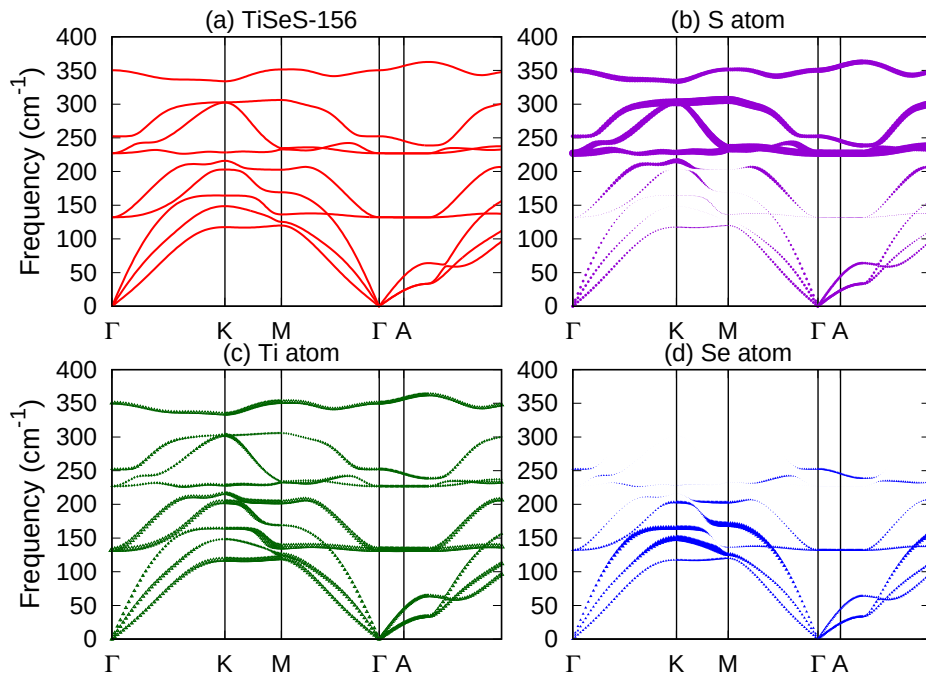


Figure S5: (color online) Atom-resolved phonon dispersions of the TiSeS-156. Contribution of atom-resolved phonon dispersion, (a) All atoms, (b) S atom, (c) Ti atom, and (d) Se atom.

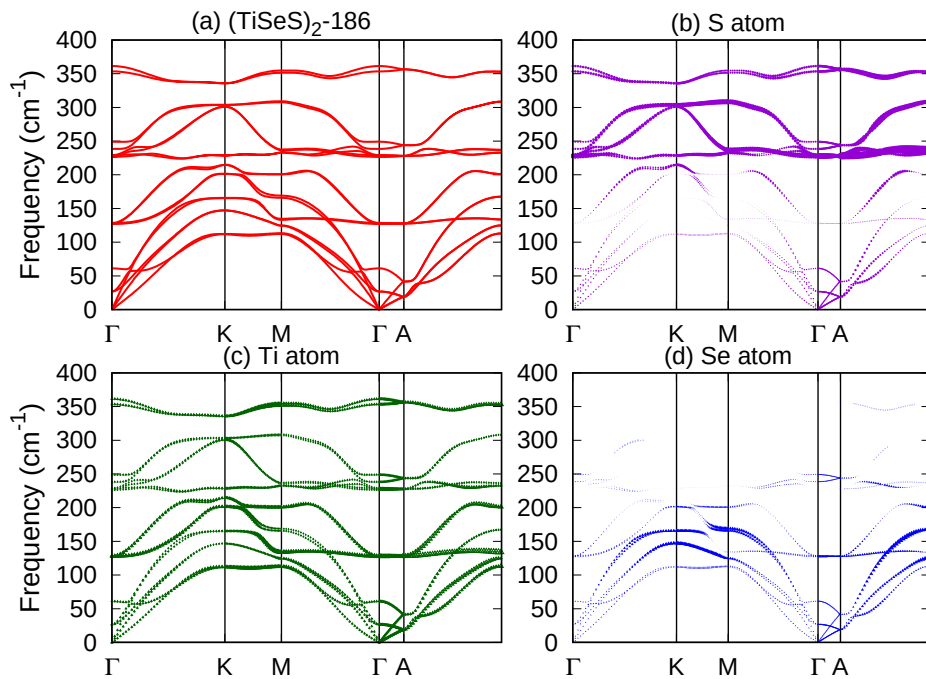


Figure S6: (color online) Atom-resolved phonon dispersions of the  $(\text{TiSeS})_2$ -186. Contribution of atom-resolved phonon dispersion, (a) All atoms, (b) S atom, (c) Ti atom, and (d) Se atom.

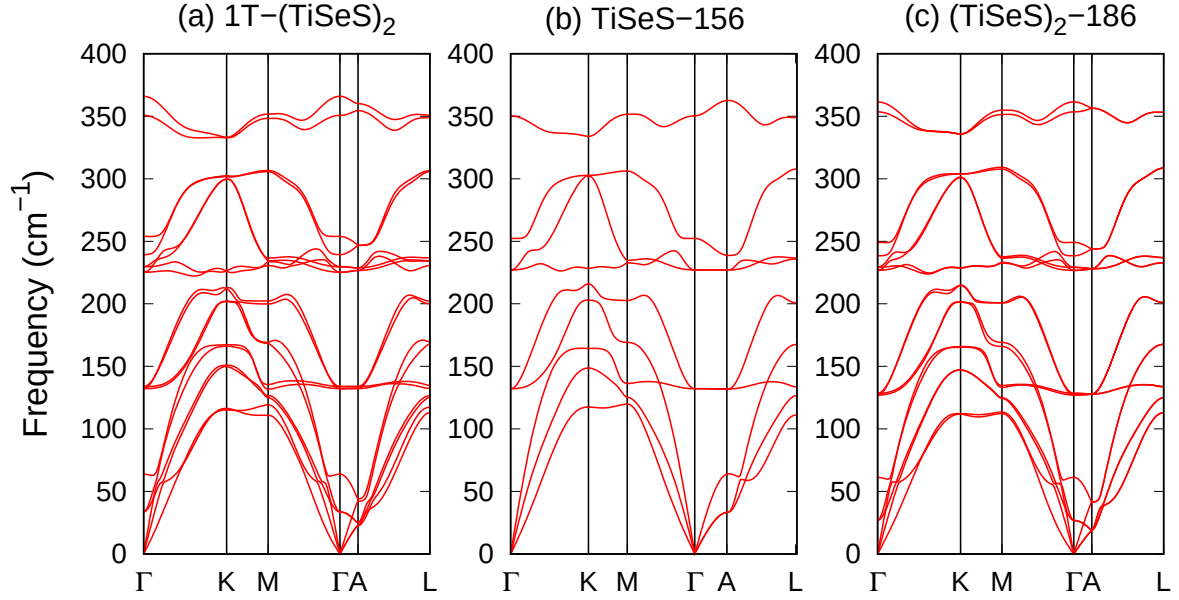


Figure S7: (color online) Phonon dispersions of (a) 1T-(TiSeS)<sub>2</sub>, (b) TiSeS-156, and (c) (TiSeS)<sub>2</sub>-186.

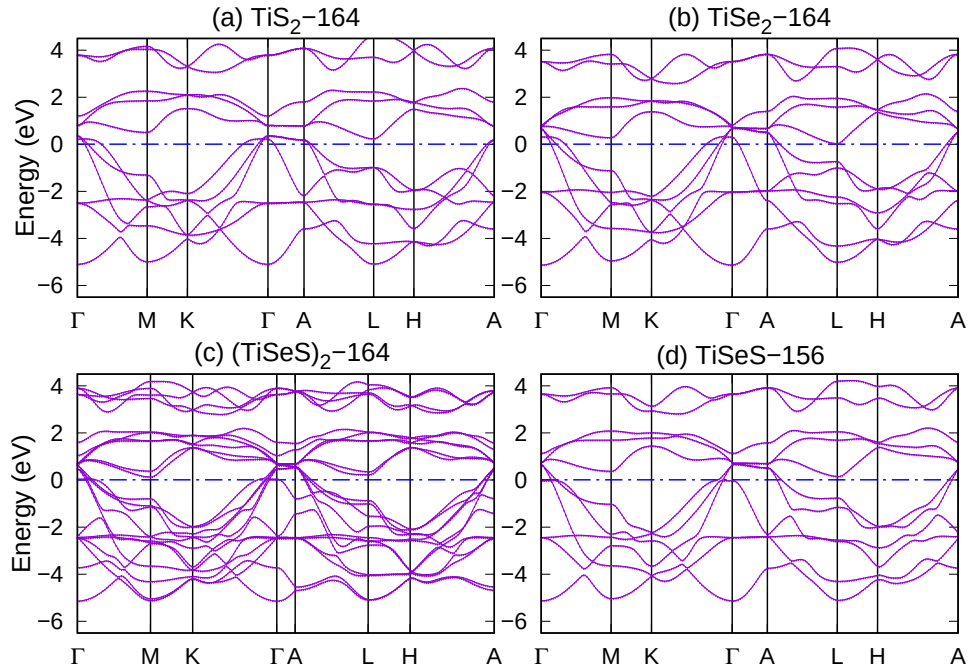


Figure S8: (color online) PBE+vdW-DF band structures for (a) 1T-TiS<sub>2</sub>, (b) 1T-TiSe<sub>2</sub>, (c) 1T-(TiSeS)<sub>2</sub> and (d) TiSeS-156.

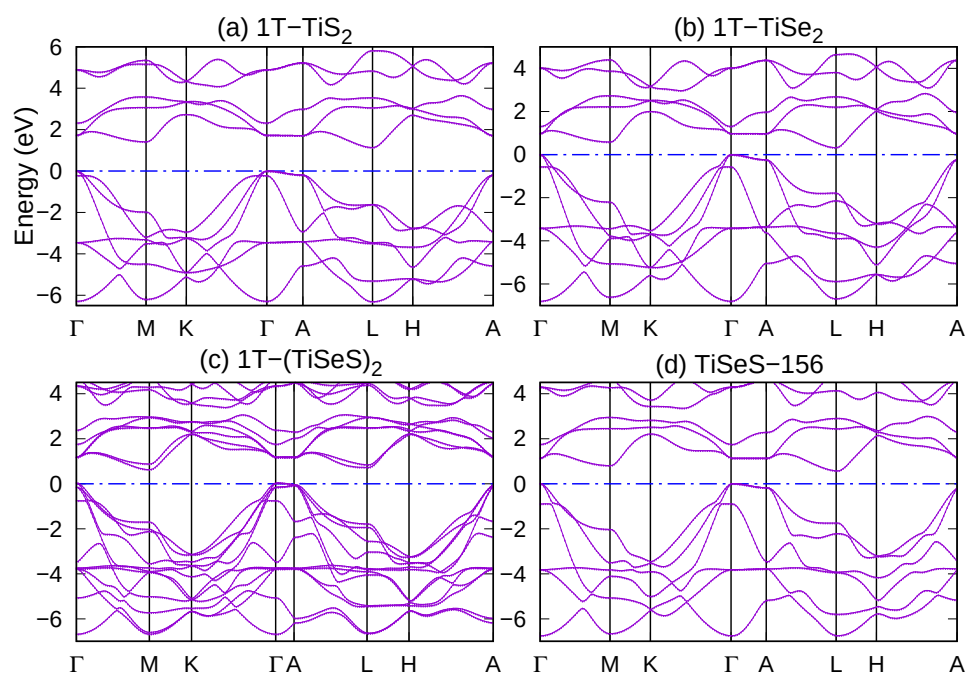


Figure S9: (color online) PBE0+vdW-DF band structures for (a) 1T-TiS<sub>2</sub>, (b) 1T-TiSe<sub>2</sub>, (c) 1T-(TiSeS)<sub>2</sub> and (d) TiSeS-156.

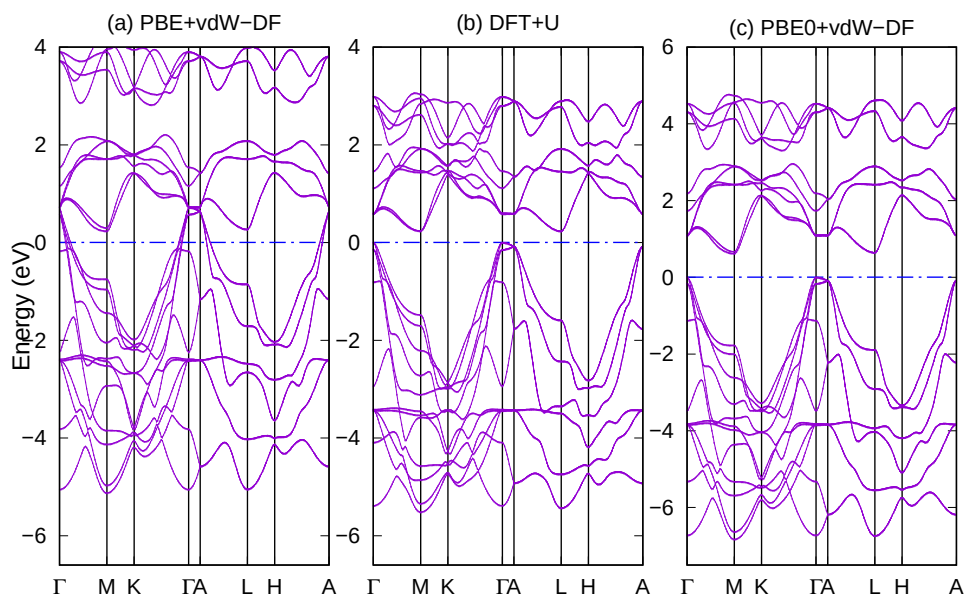


Figure S10: (color online) PBE+vdW-DF, DFT+U, and PBE0+vdW-DF band structures for (TiSeS)<sub>2</sub>-186.

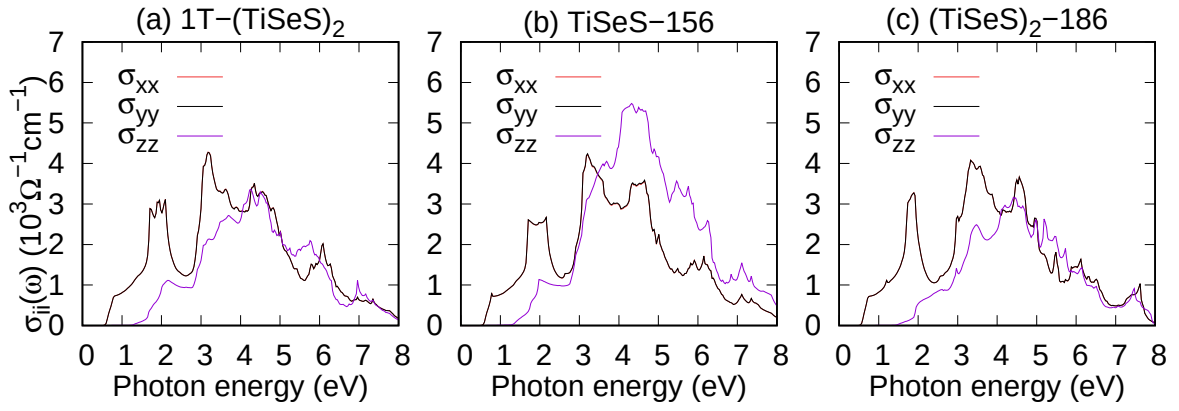


Figure S11: (color online) Optical conductivity  $\sigma_{ii}(\omega)$  of (a) 1T-(TiSeS)<sub>2</sub>, (b) TiSeS-156, and (c) (TiSeS)<sub>2</sub>-186, where  $\omega$  is the photon energy and  $i = x, y, z$ .