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

Two-dimensional Janus Si dichalcogenides: A first-principles study

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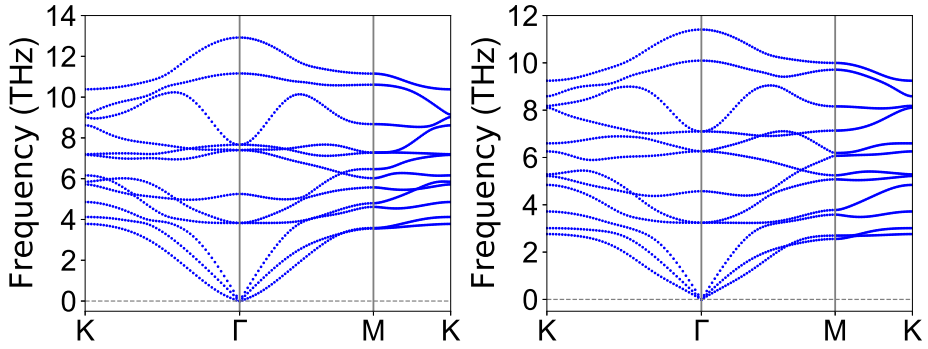

FIG. 1. (Color online)The phonon band dispersions of Si_2SSe (left) and Si_2STe (right).

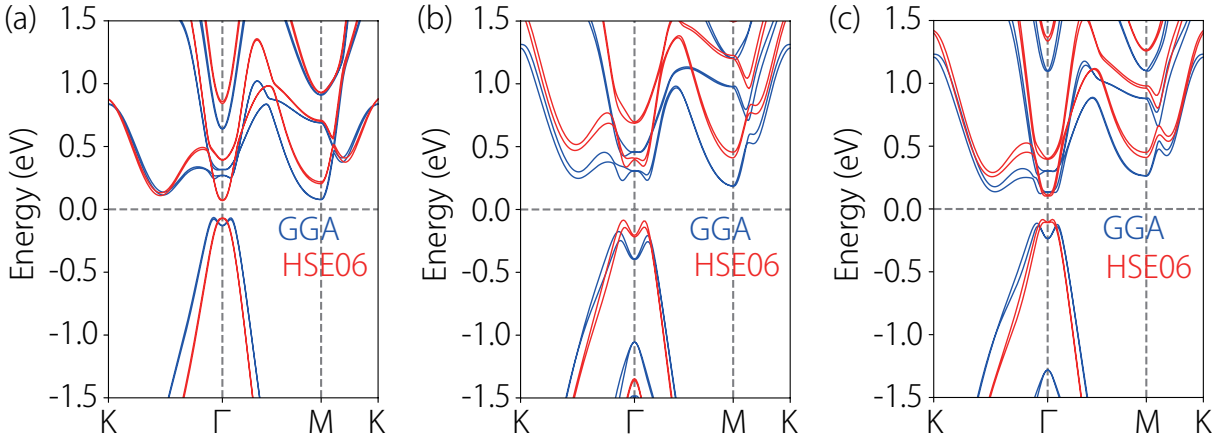

FIG. 2. (Color online)Comparison of band structures obtained by HSE06 and PBE: (a) Si_2SSe, (b) Si_2STe, and (c) Si_2SeTe. Note: for the HSE06 calculations, the parameter ISYM=3 is set.

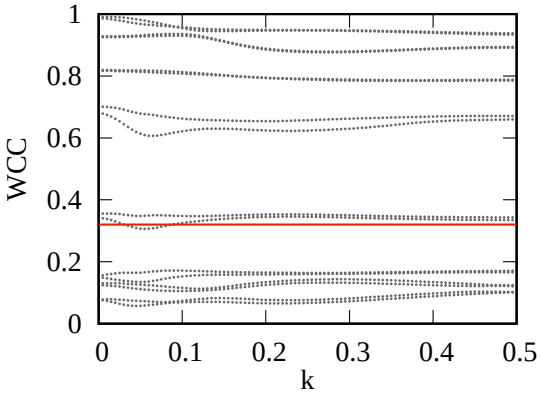

FIG. 3. (Color online)For monolayer Si_2SeTe, the evolution of WCC, and an arbitrary reference line crosses the evolution lines of WCC twice time, giving rise to $\mathbb{Z}_2$=0.

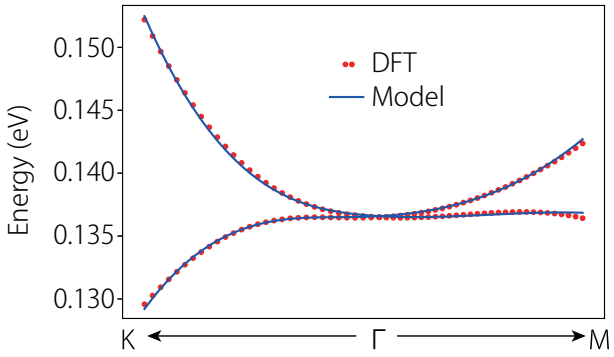

FIG. 4. (Color online)Comparison of DFT band structure with the model fitting.

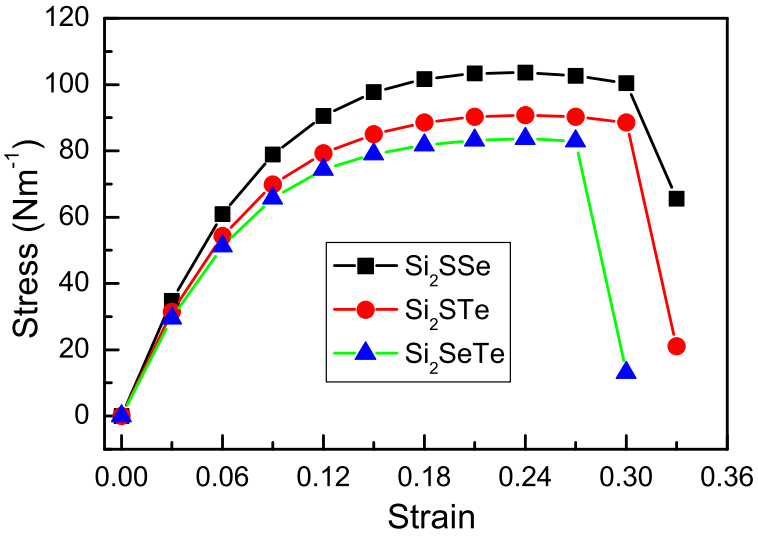

FIG. 5. (Color online)Stress-strain relationships of monolayer JSD materials under biaxial tensions.

TABLE I. Comparison of band gap values obtained by PBE and HSE06 approaches (unit: meV).

Name	PBE+SOC	HSE06+SOC
Si_2SSe	142	139
Si_2STe	361	422
Si_2SeTe	235	186