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Supplementary information

Strain-induced phase transitions and high carrier mobility in two-dimensional Janus MGeSN$_2$ (M = Ti, Zr, and Hf) structures: First-principles calculations

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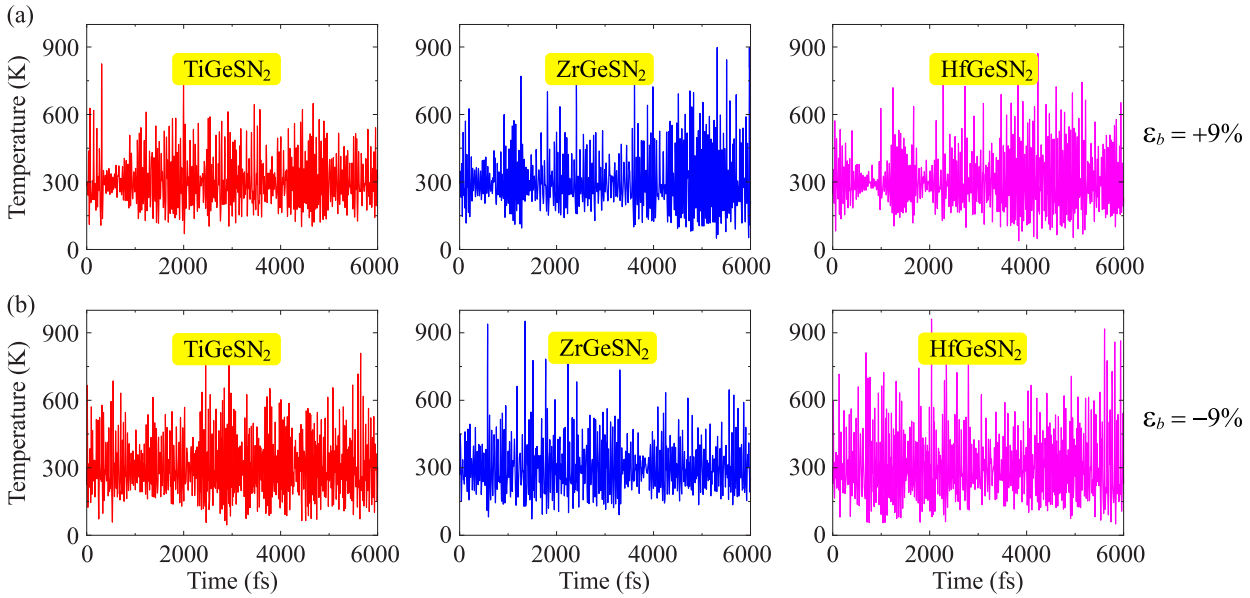

Fig. S1. AIMD simulations for temperature fluctuations to simulation time at 300 K of strained MGeSN$_2$ monolayers at $\varepsilon_b = +9\%$ (a) and $\varepsilon_b = -9\%$ (b).

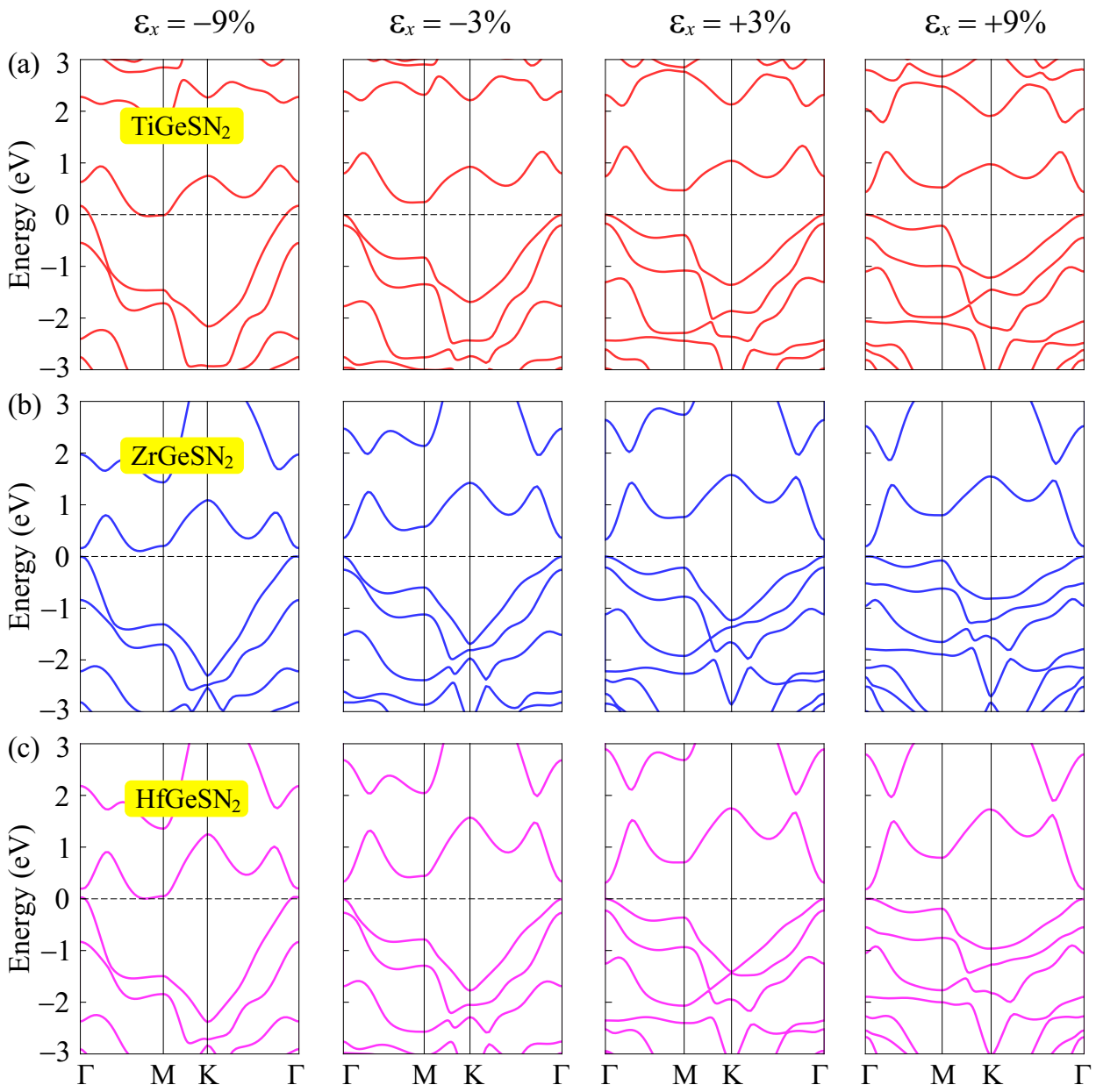

Fig. S2. Band structures of (a) $TiGeSN_2$, (b) $ZrGeSN_2$, and (c) $HfGeSN_2$ under a uniaxial strain along the x-axis ε_x.

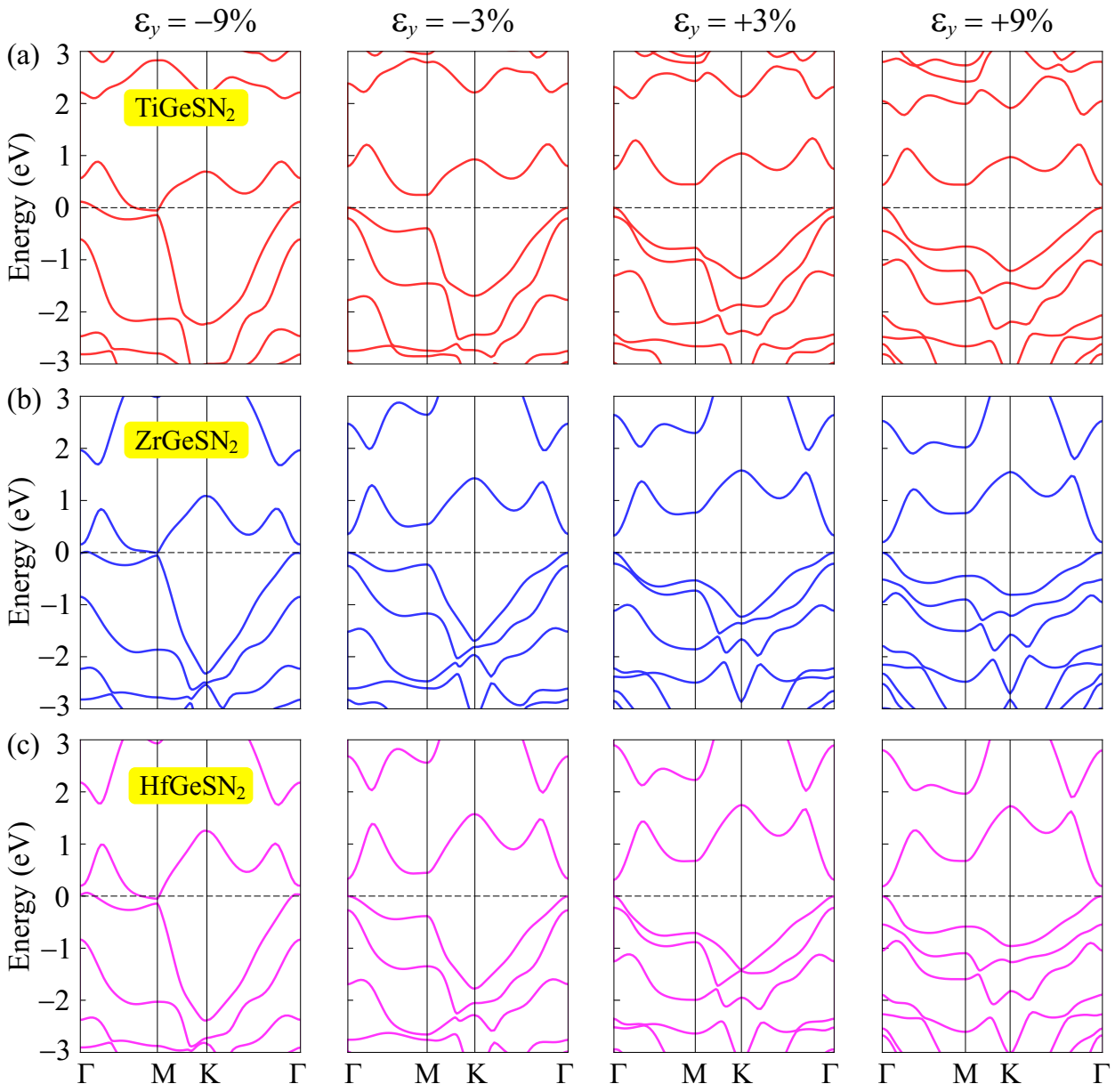

Fig. S3. Band structures of (a) $TiGeSN_2$, (b) $ZrGeSN_2$, and (c) $HfGeSN_2$ under a uniaxial strain along the y-axis ε_y.