Supporting Information

Monolayer SnI_2: an excellent p-type thermoelectric material with ultralow lattice thermal conductivity

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The Thermal Stability

The thermodynamic stability of the 2D system is of great importance. We run the ab-initio molecular dynamics (AIMD) simulations at 800 K for SnI_2 monolayers. Results show that SnI_2 monolayer can be maintained up to 10 ps at 800 K, suggesting they are stable at high temperature.

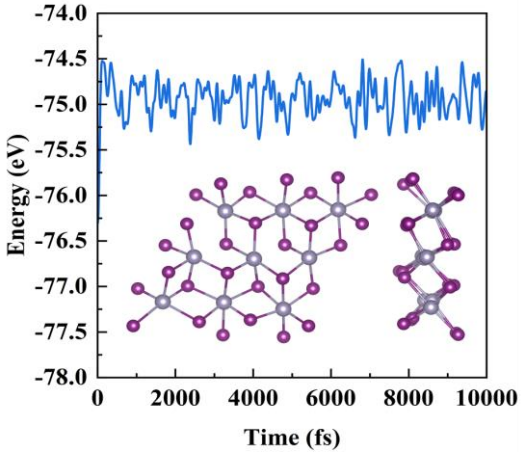

Figure S1. Free energy fluctuations with respect to time and equilibrium structures of SnI_2 monolayer by AIMD simulations at 800 K.