

Theoretical insight into the thermoelectric transport performance of MoP₂Ga₂S₂ monolayer

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1. The AIMD stimulation for MoP₂Ga₂S₂ monolayer at 1500 K.

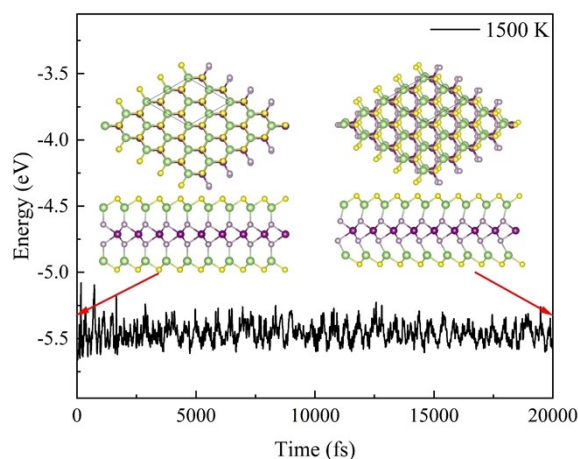


Fig. S1 The ab-initio molecular dynamics (AIMD) simulation results of $\text{MoP}_2\text{Ga}_2\text{S}_2$ monolayer at 1500 K. The AIMD runs for 20 ps with a time step of 1 fs.

2. The energy band structures of monolayer $\text{MoP}_2\text{Ga}_2\text{S}_2$ using PBE, PBE+SOC and HSE06

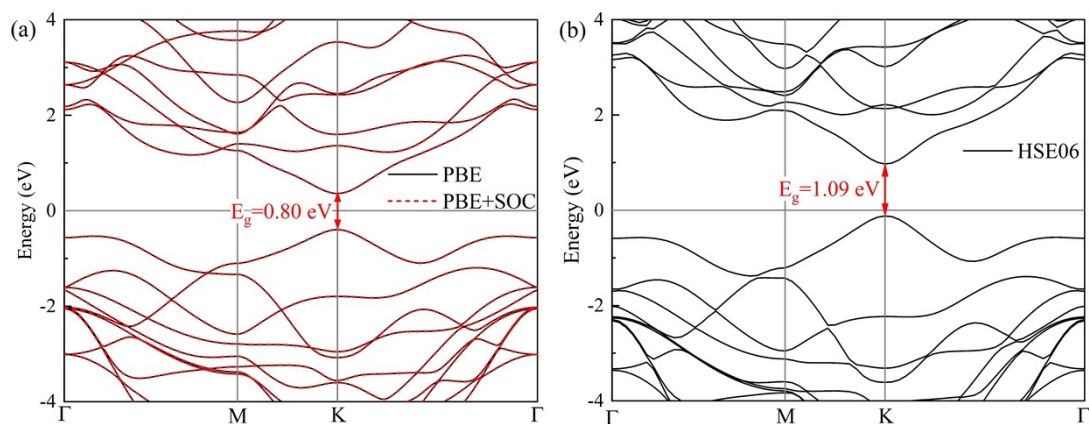


Fig. S2 The energy band structure using (a) PBE and PBE+SOC, (b) HSE06 of $\text{MoP}_2\text{Ga}_2\text{S}_2$ monolayer.

3. The boundary scattering rate and isotopic scattering rate in the irreducible wedge of $\text{MoP}_2\text{Ga}_2\text{S}_2$ monolayer

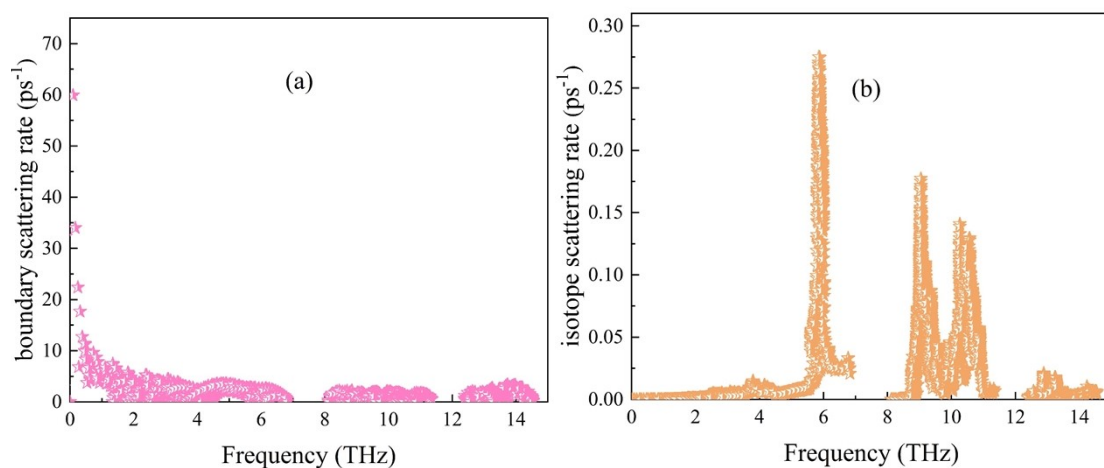


Fig. S3 (a) The boundary scattering rate and (b) isotopic scattering rate of $\text{MoP}_2\text{Ga}_2\text{S}_2$ monolayer.