

Supplementary Information

Enhanced thermoelectric performance and reversed anisotropy in Janus penta-PdSeTe monolayer via biaxial strain

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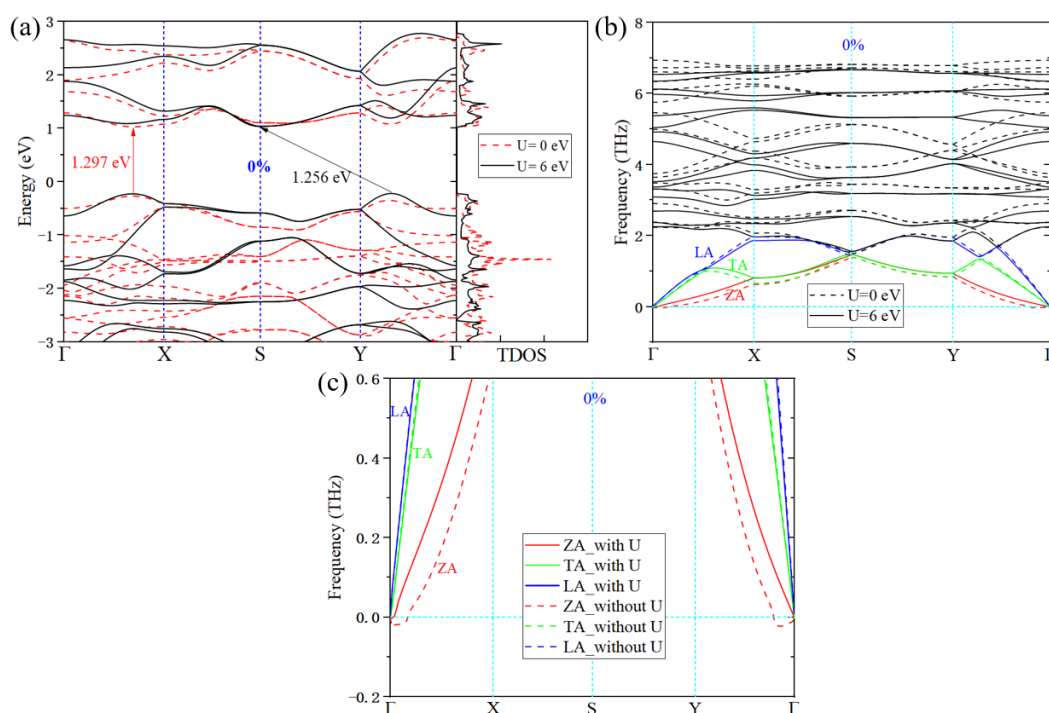


Fig. S1 Band structure (a) and phonon spectrum (b) within PBE and PBE+U for penta-PdSeTe monolayer. The enlarged phonon spectrum (c) is also presented in order to clearly show the imaginary frequency without U.

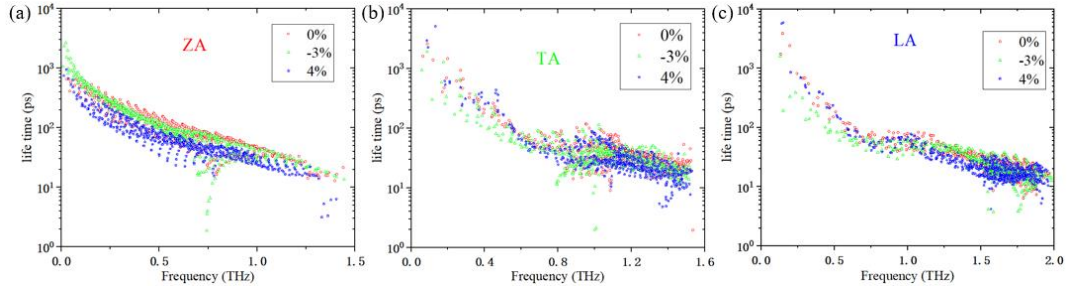


Fig. S2 The phonon life time of ZA (a), TA (b), LA (c) branches at 300 K for PdSeTe monolayer under different strains.

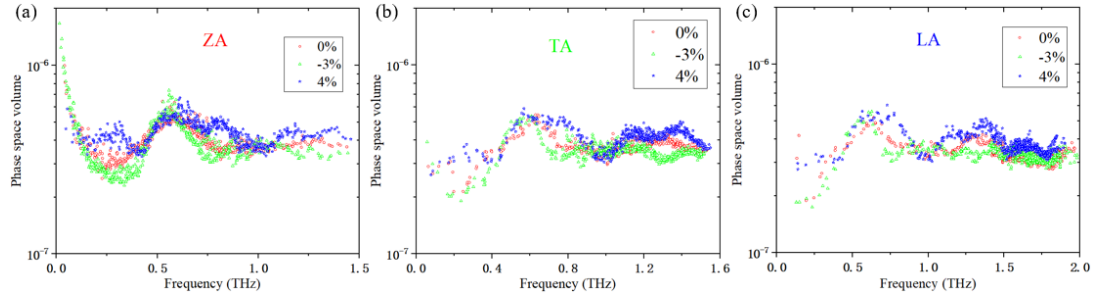


Fig. S3 The phase space volume of ZA (a), TA (b), LA (c) branches at 300 K for PdSeTe monolayer under different strains.