

Ultra-high thermoelectric performance of Janus α -STe₂ and SeTe₂ monolayers

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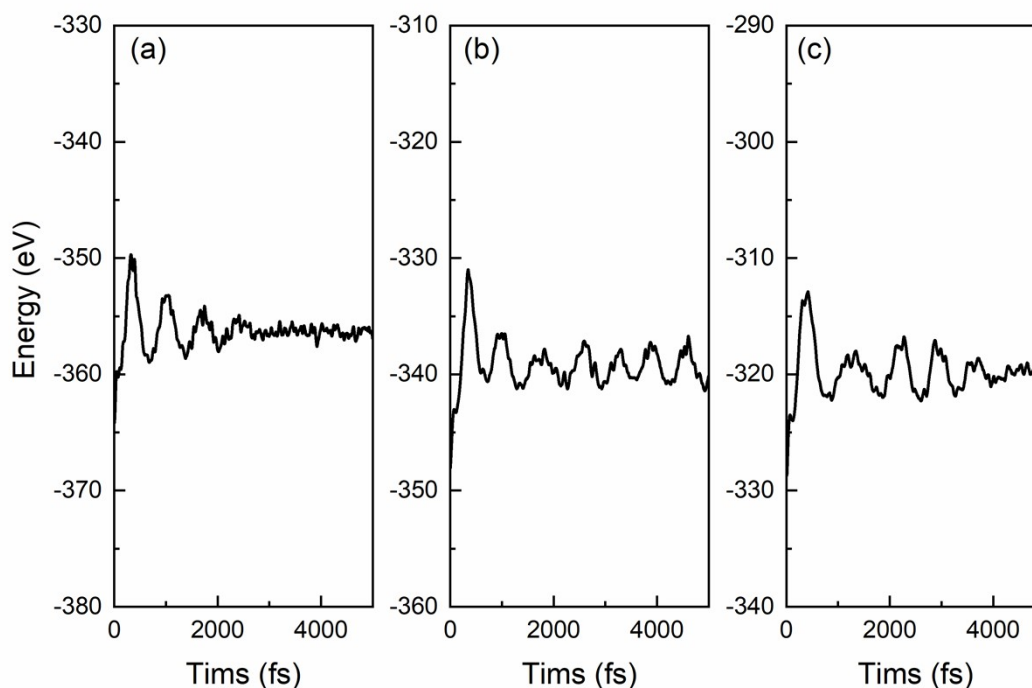


Fig. S1. AIMD simulation curves of energy with respect to time for (a) α -STe₂, (b) α -SeTe₂ and (c) α -Te monolayers at 500 K. The energy curves fluctuate, but the average energies remain nearly invariant, confirming the thermal stabilities of the three monolayers at 500 K.