

## Supplementary Material

### Two-dimensional $\alpha$ -As/ $\alpha$ -AsP van der Waals heterostructure for photovoltaic applications

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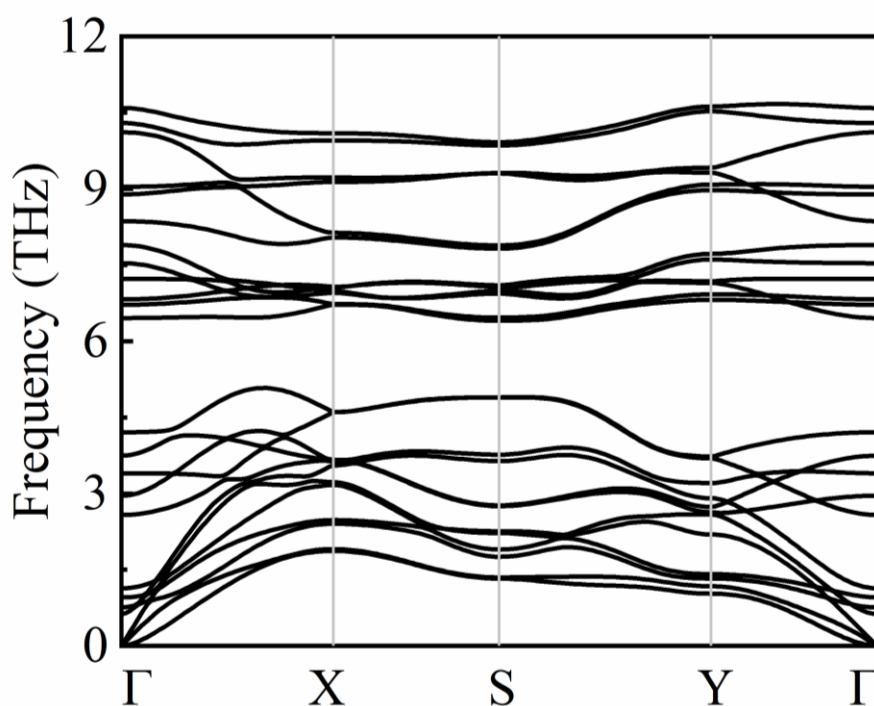
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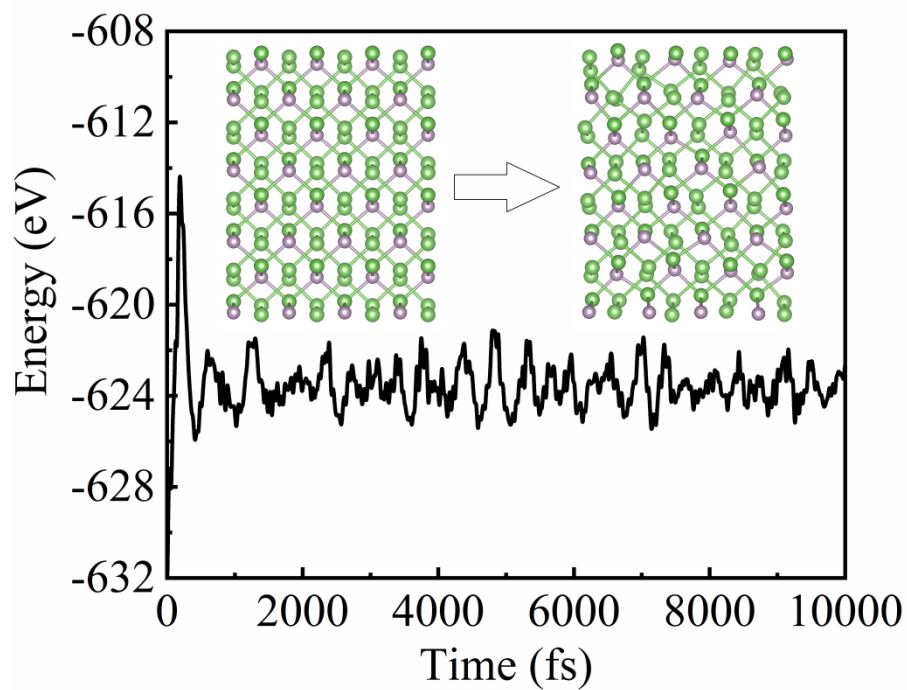
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1. Phonon dispersion of AB stacking two-dimensional  $\alpha$ -As/ $\alpha$ -AsP van der Waals heterostructure under 300 K.



**Fig. S1** Phonon dispersion of AB stacking two-dimensional  $\alpha$ -As/ $\alpha$ -AsP van der Waals heterostructure under 300 K.

2. Total energy fluctuations in the MD simulations under 500K.



**Fig. S2** Total energy fluctuations in the MD simulations under 500K. The insets show snapshots of the structures after 10000 fs.