

## Supporting Information

### Transition Metal Si-Chalcogenides: A New Two-Dimensional Anode Material for Na-Ion Batteries

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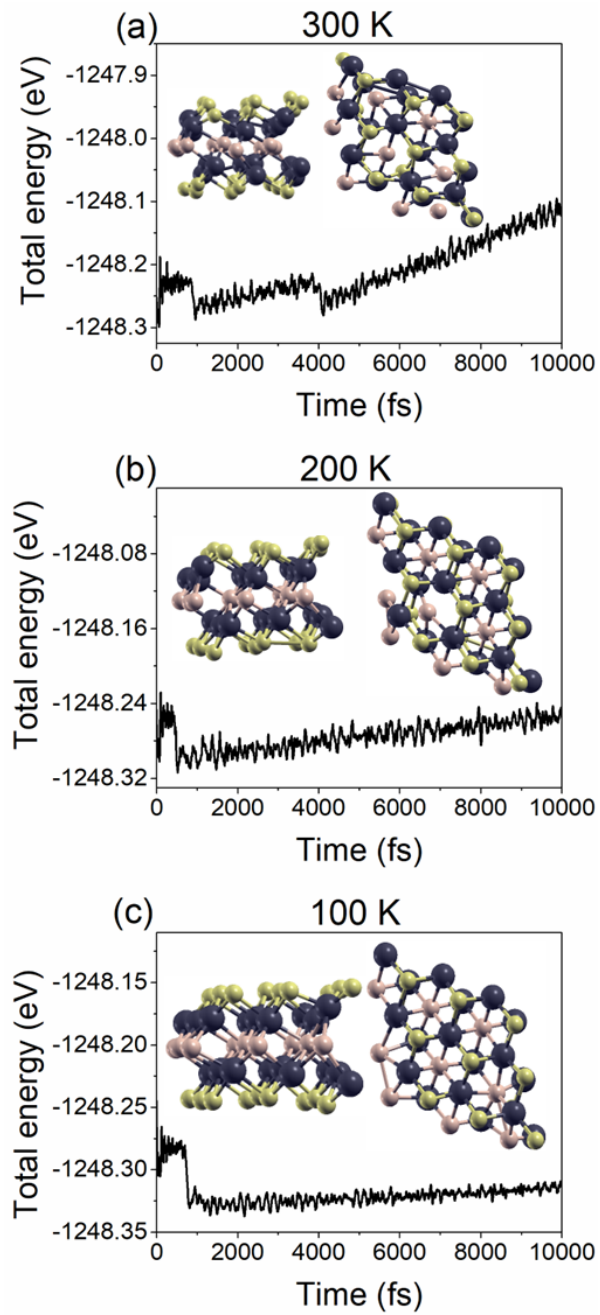
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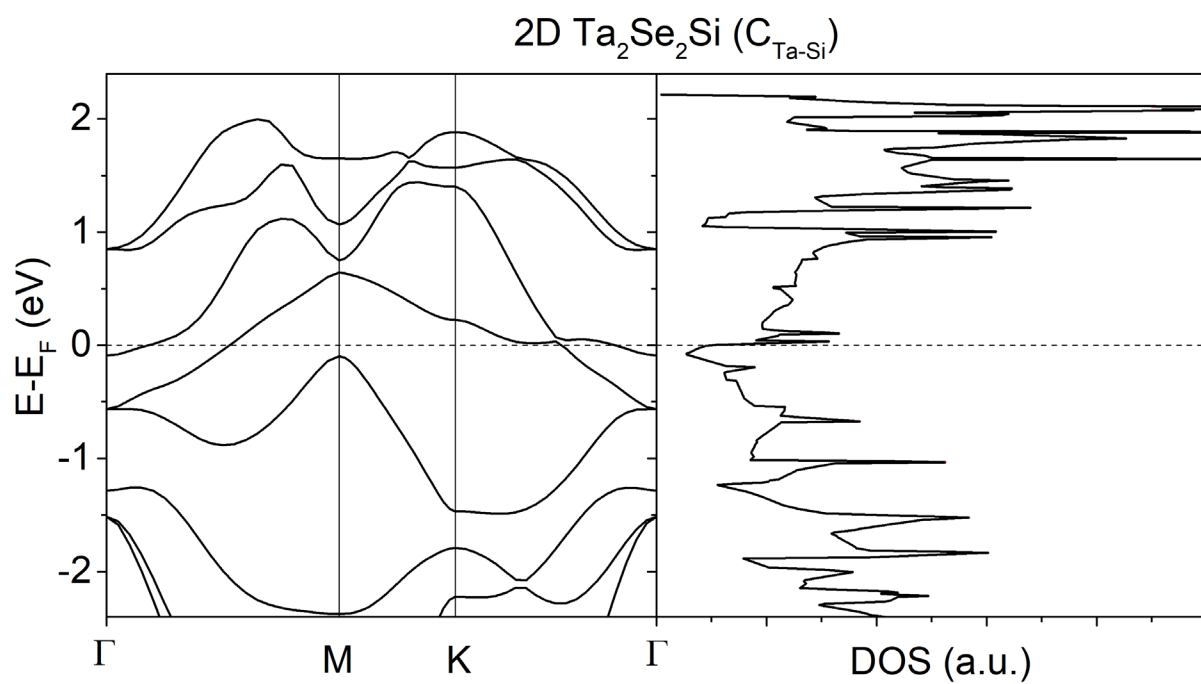
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**Fig. S1** Fluctuation of energy under AIMD simulations at (a) 300 K (b) 200 K and (c) 100 K for 2D Nb<sub>2</sub>S<sub>2</sub>Si. The yellow, black and light pink balls denote S, Nb and Si atoms, respectively.



**Fig. S2** Band structure and DOS of the 2D  $\text{Ta}_2\text{Se}_2\text{Si}$  ( $C_{\text{Ta-Si}}$ ).