

Supporting Information

Mechanisms of Semiconducting 2H to Metallic 1T Phase Transition in Two-dimensional MoS₂ Nanosheets

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Figure S1. Calculated phase transition mechanisms for the Mo edge with 100%S.

Figure S2. Optimized edges of 2H-MoS₂. (a) Mo-edge with 0% S coverage; (b) Mo-edge with 50% S coverage; (c) S-edge with 50% S coverage; (d) S-edge with 100% S coverage.

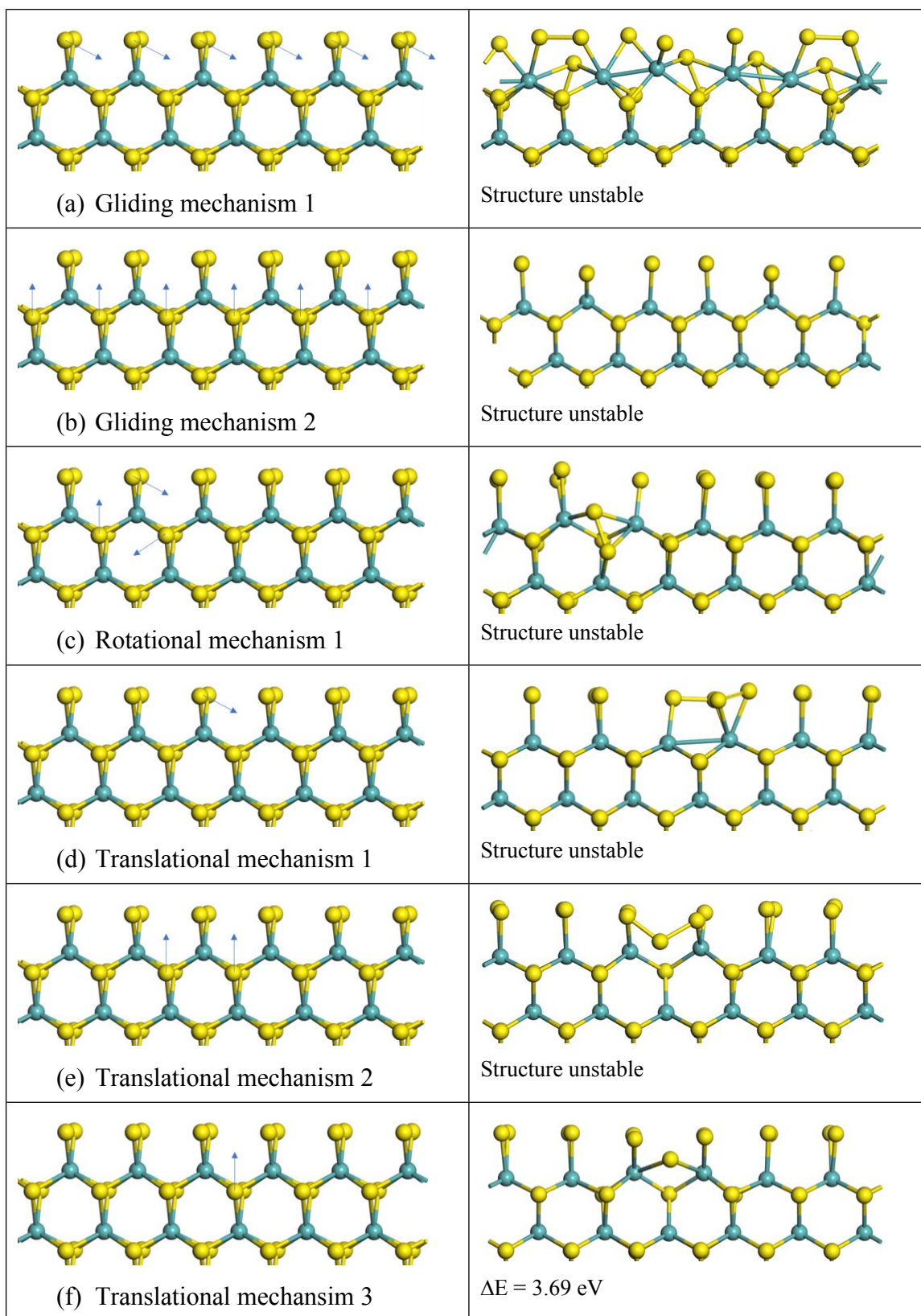


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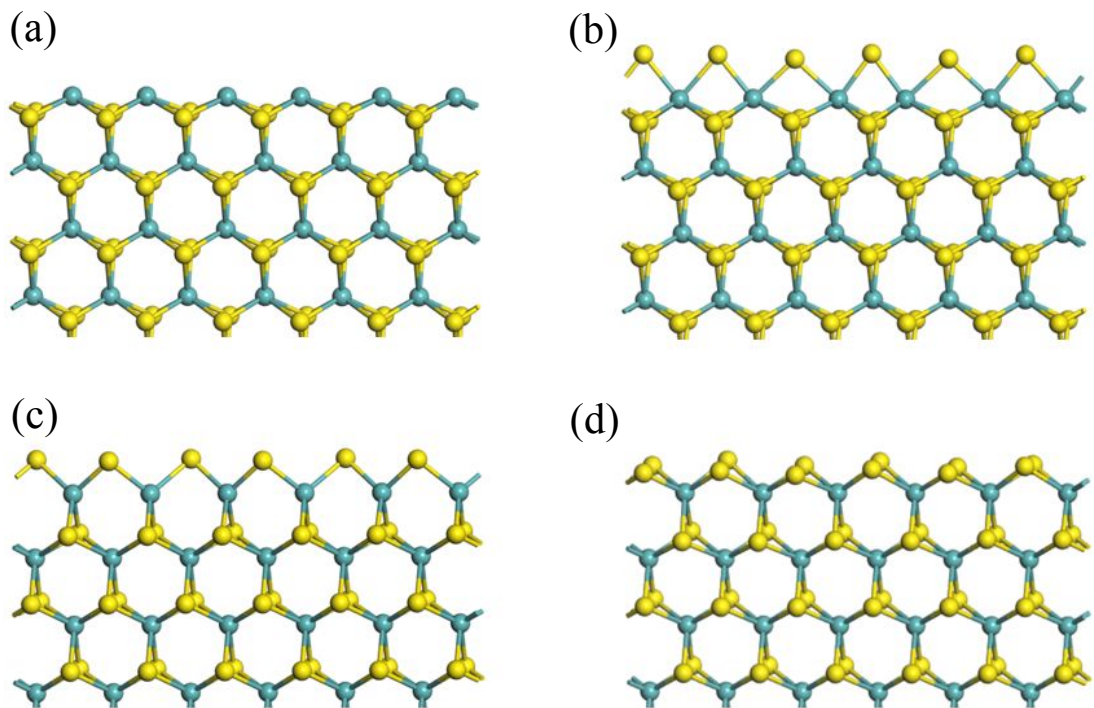


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