

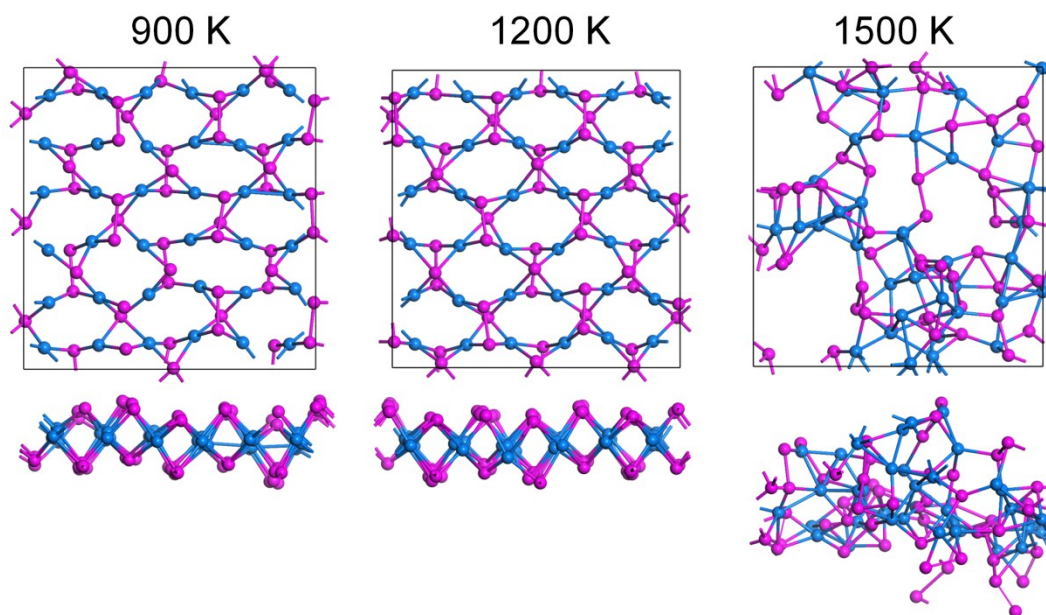
Electronic Supplementary Information

**Pd<sub>2</sub>Se<sub>3</sub> Monolayer: A Novel Two-Dimensional Material with  
Excellent Electronic, Transport, and Optical Properties**

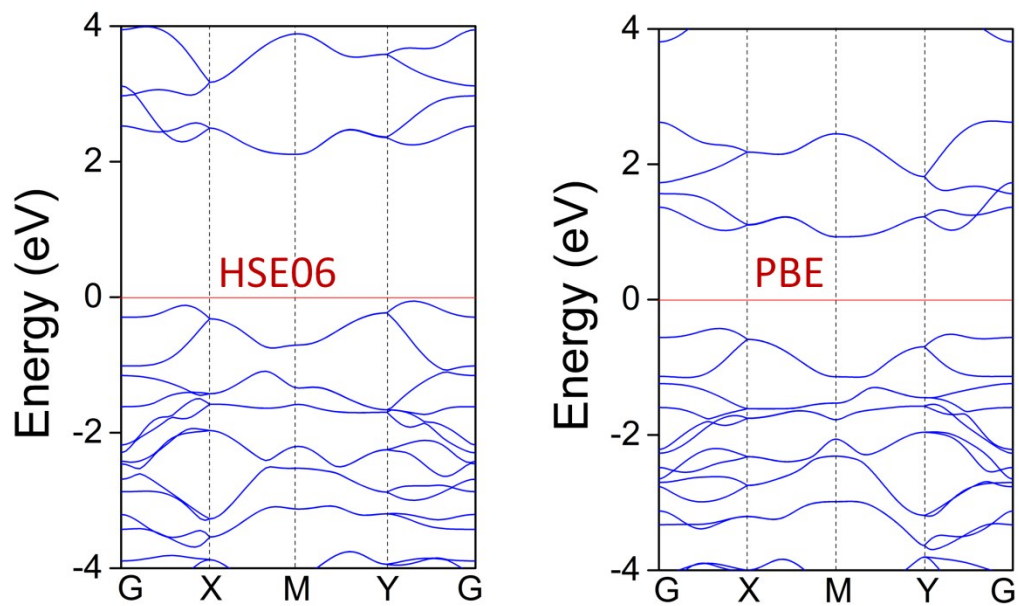
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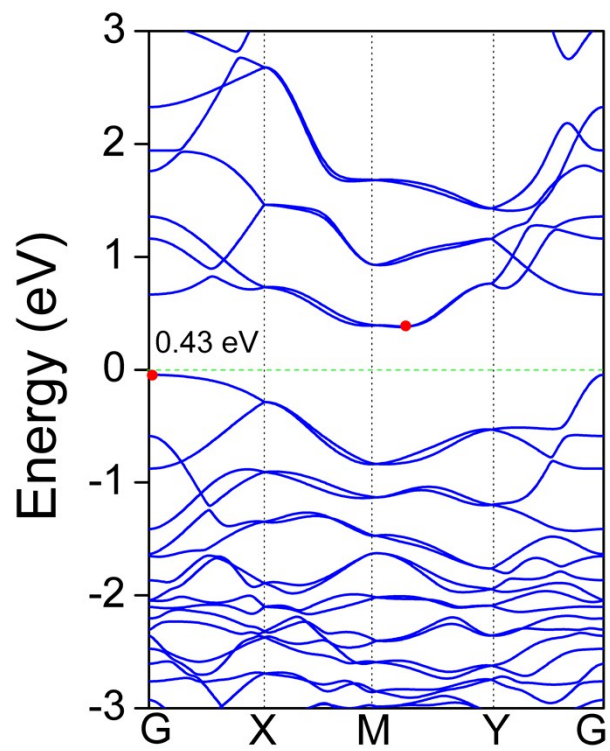
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**Fig. S1** Top and side views of snapshots of Pd<sub>2</sub>Se<sub>3</sub> monolayer equilibrium structures at 900 K (left), (b) 1200 K (middle), and (c) 1500 K (right) at the end of 10 ps first-principles molecular dynamics simulations.



**Fig. S2** Band structure of PdSe<sub>2</sub> monolayer computed using (a) HSE06 and (b) PBE functional.



**Fig. S3** Band structure of Pd<sub>2</sub>Se<sub>3</sub> monolayer computed using PBE functional including spin-orbital coupling (SOC).