Supplementary Information

Hydrogen-Induced Tunable Electronic and Optical Properties of Two-Dimensional Penta-Pt_2N_4 Monolayer

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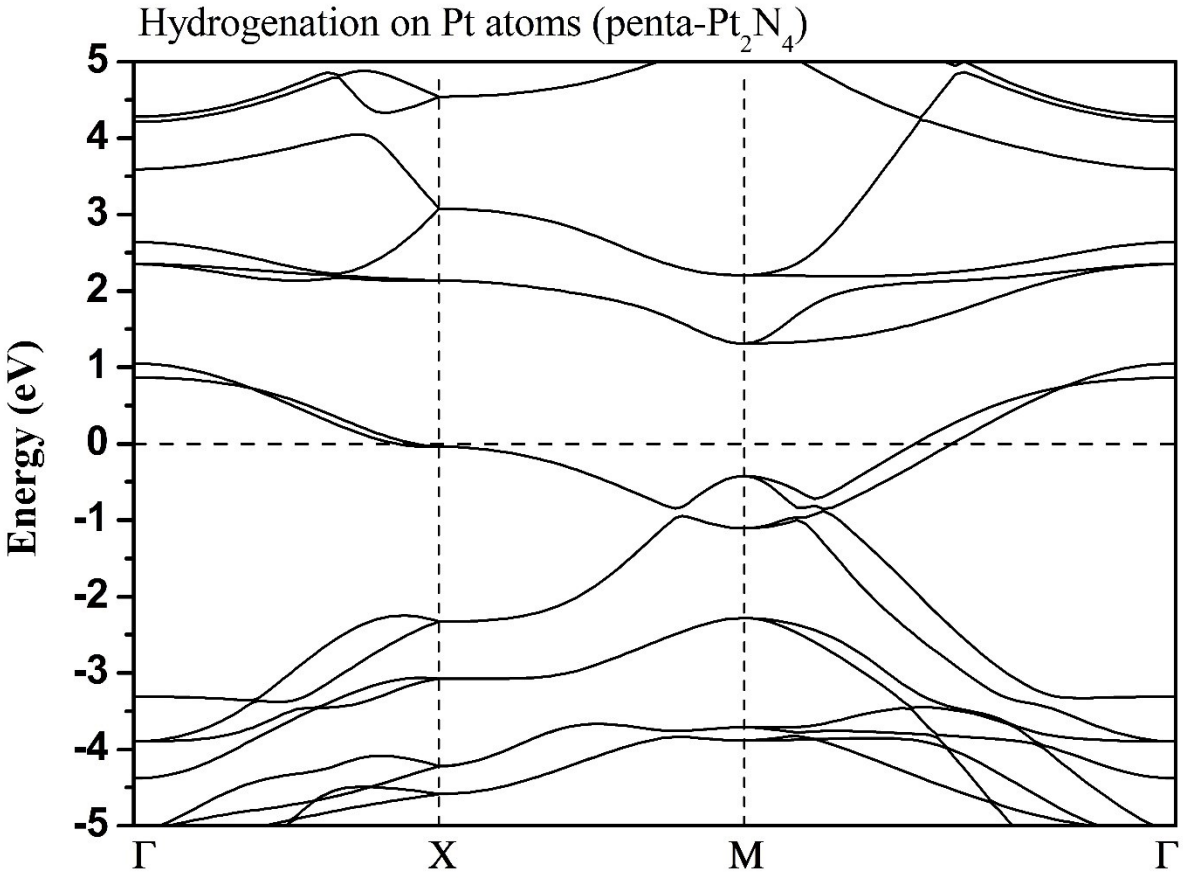

Figure S1. The band diagram of hydrogenation on Pt atoms (penta-Pt_2N_4)

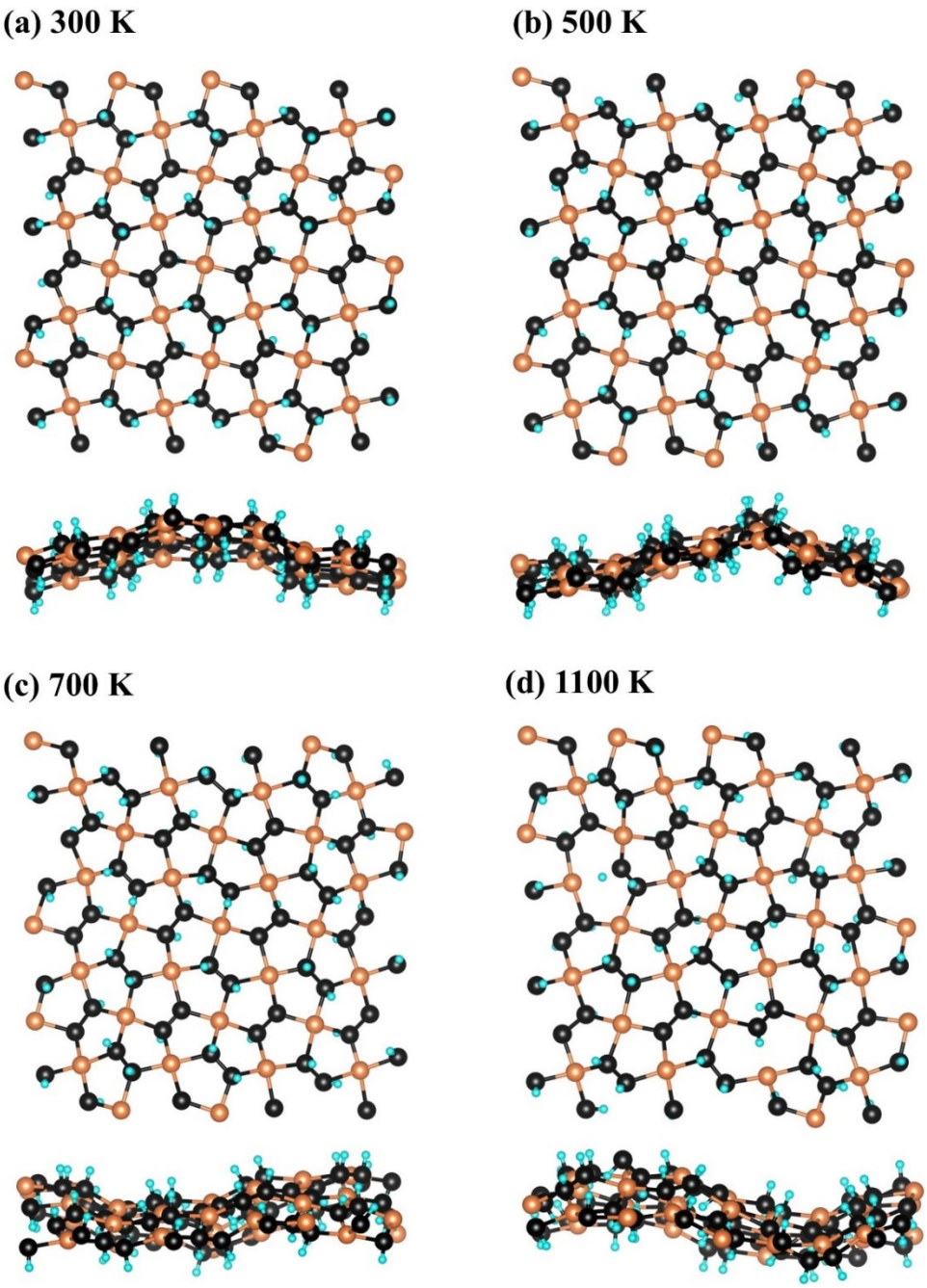

Figure S2. The snapshots of hydrogenated Pt_2N_4 at the end of 5 ps AIMD simulations at 300 K, 500 K, 700 K, and 1100 K.

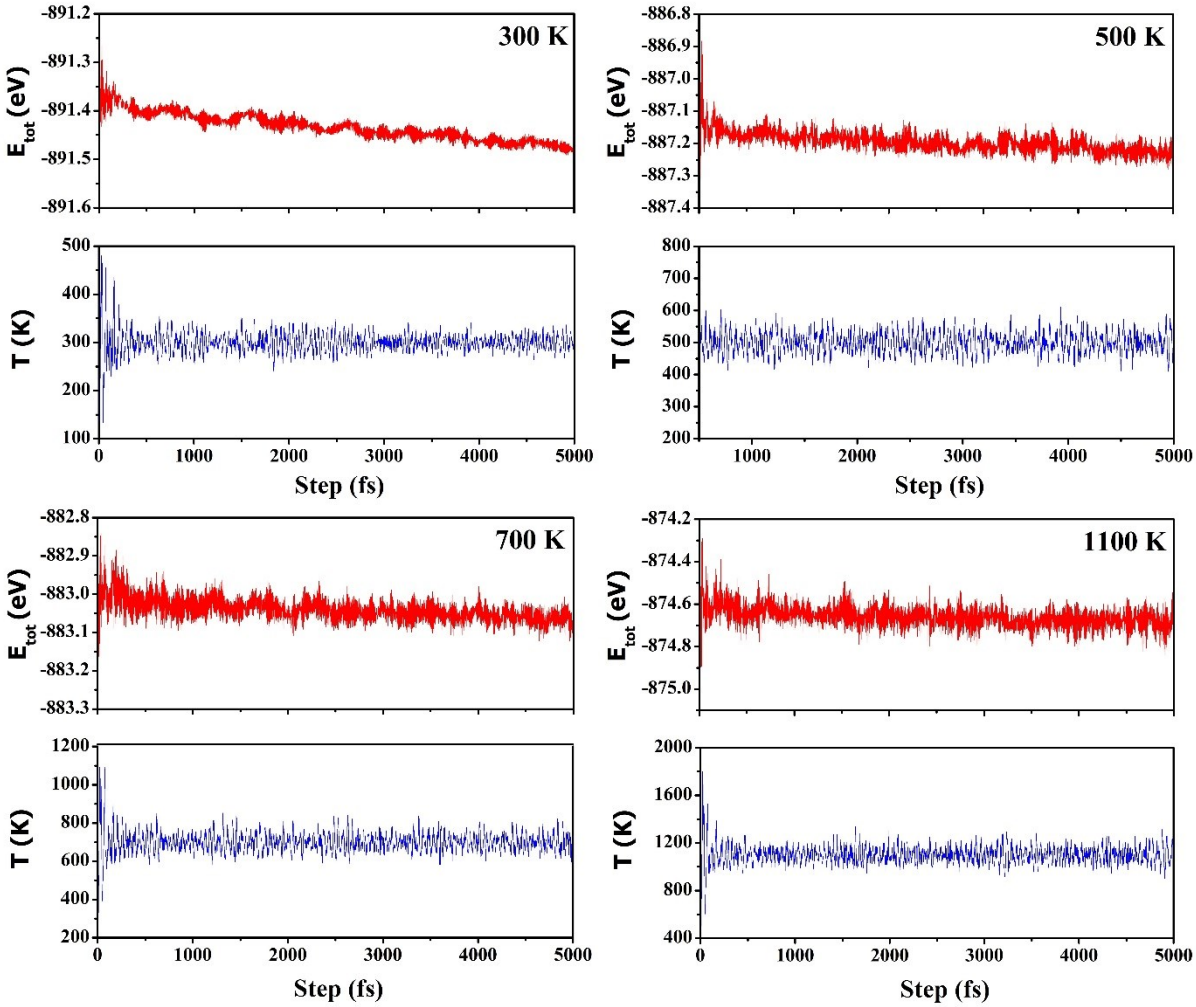

Figure S3. Fluctuation in total potential energy and temperature during the AIMD simulation of hydrogenated Pt_2N_4 at temperatures of 300 K, 500 K, 700 K, and 1000 K.

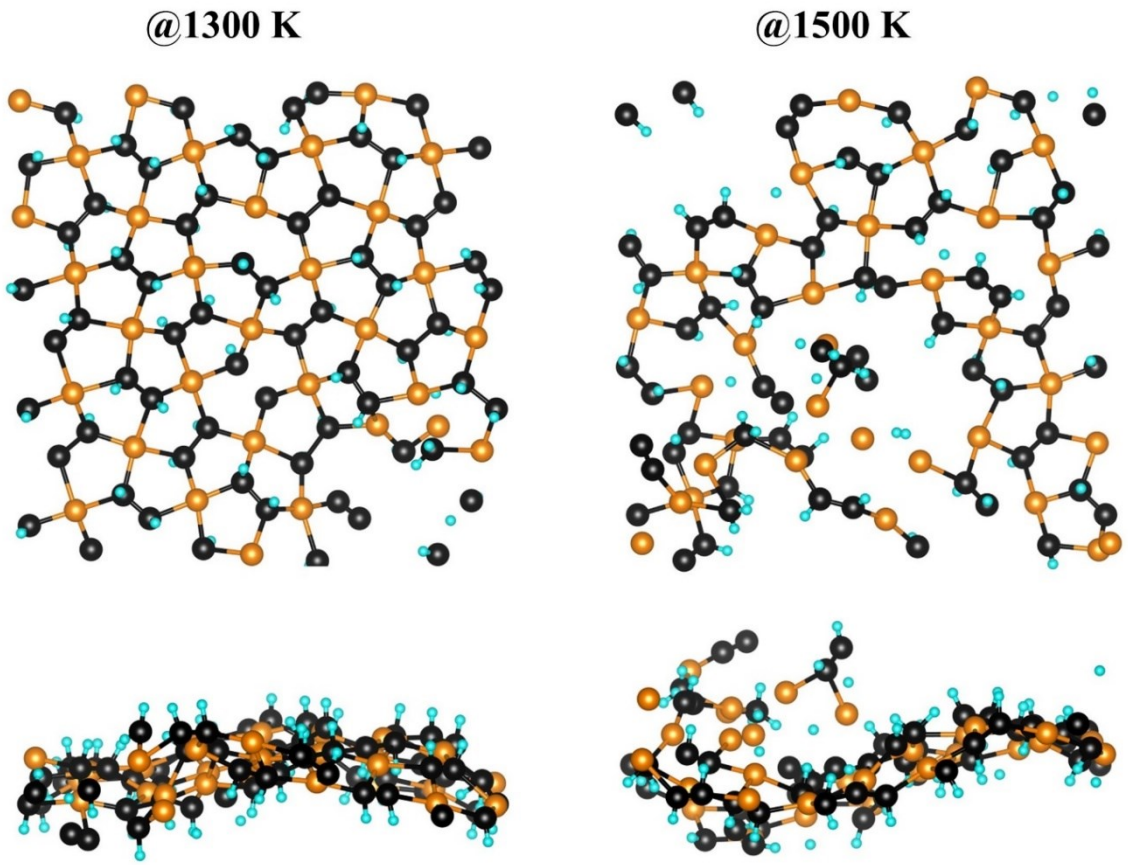

Figure S4. The snapshots of hydrogenated Pt_2N_4 at the end of 5 ps AIMD simulations at 1300 K and 1500 K.

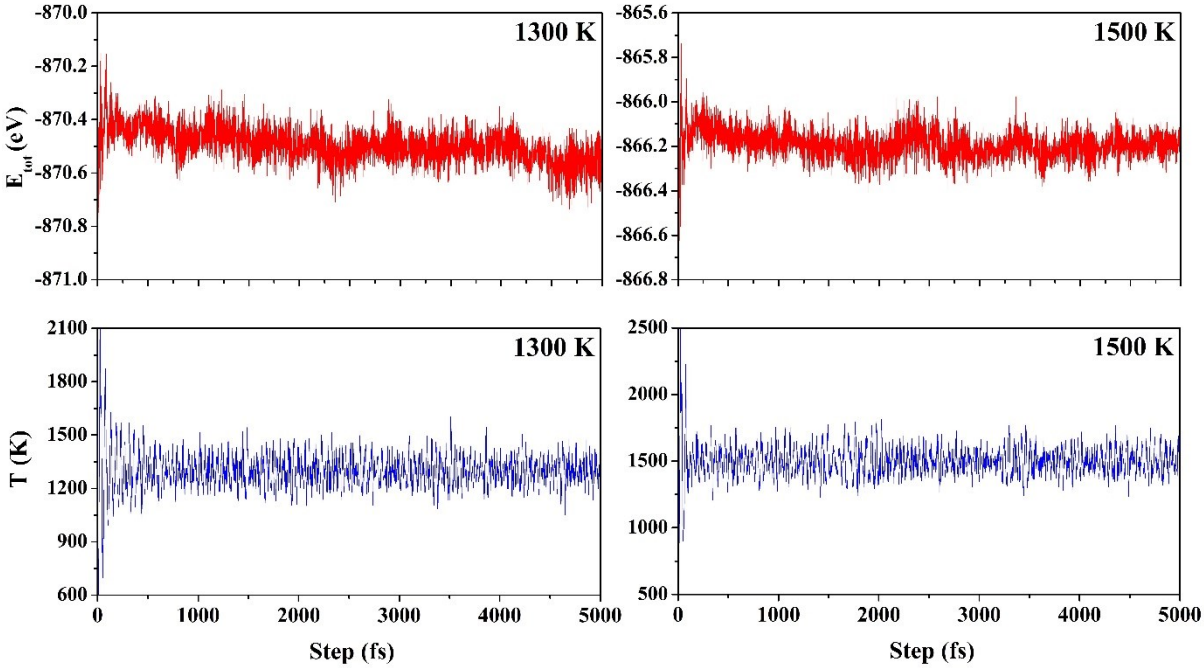

Figure S5. Fluctuation in total potential energy and temperature during the AIMD simulation of hydrogenated Pt_2N_4 at 1300 K and 1500 K.