Electronic Supplementary Information for

Edge-State-induced Magnetism in two-dimensional Hematene

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This file includes:

Fig. S1 Stability analysis of the 2D hematene crystal. (a) Phonon spectrum; (b)-(d) Structural snapshots of 2D hematene crystal at time of 10 ps during AIMD simulation under the temperatures of 300, 900, and 1500 K, respectively.

Fig. S2 Lattice constant as a function of the values of Hubbard U_{eff} in DFT+U calculations.

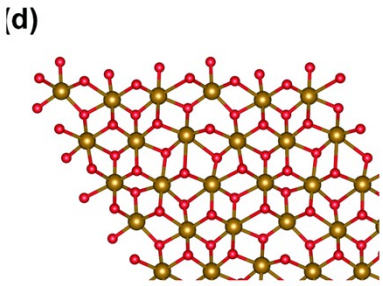

Fig. S1 Stability analysis of the 2D hematene crystal. (a) Phonon spectrum; (b)-(d) Structural snapshots in both top and side views of the 2D hematene crystal at time of 10 ps during AIMD simulation under the temperatures of 300, 900, and 1500 K, respectively.

As shown in Fig. S1, from both the phonon calculation and the AIMD simulations, one can conclude that the present 1T structure is a real local minim. Particularly, the AIMD calculation demonstrate the thermodynamic stability of the 1T structure at fairly high temperatures.

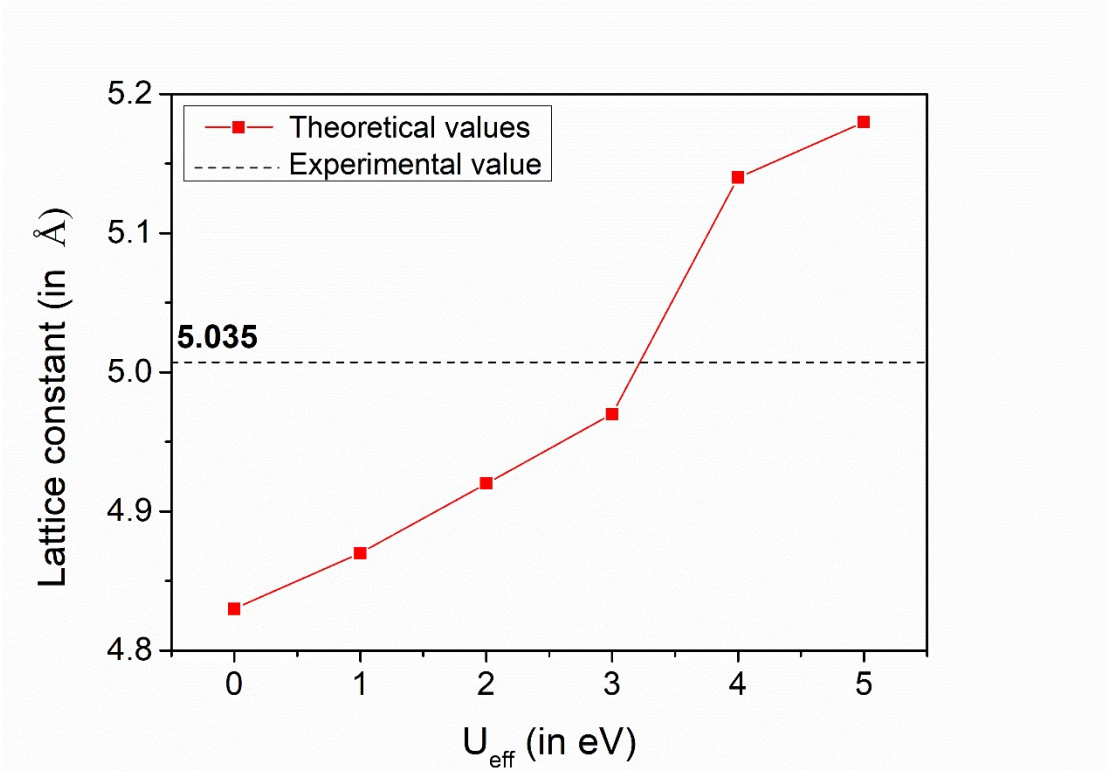

Fig. S2 Lattice constant as a function of the values of Hubbard U_{eff} in DFT+U calculations.

Based on Fig. S2, one can see that the optimum U_{eff}=3 eV is reasonably selected in the present calculations.