Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Support Information

Diamondization of Graphene and Graphene-BN Bilayers: Chemical Functionalization and Electronic Structure Engineering

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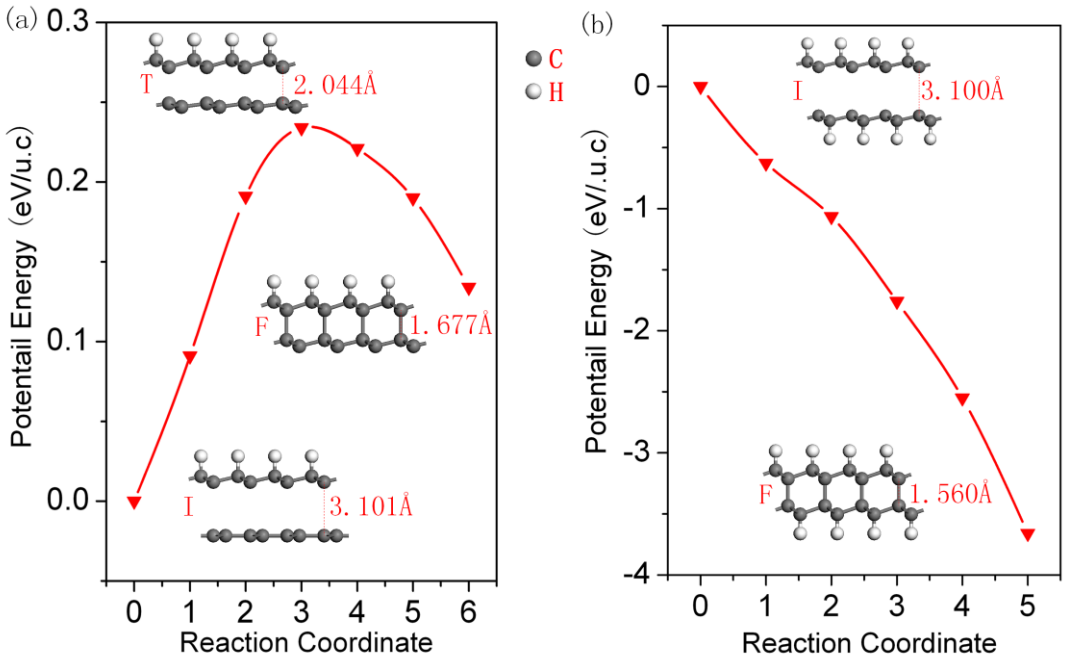

Fig. S1. Minimum energy path for transition processes (a) from single-side functionalized bilayer to diamondized film, (b) from double-side functionalized bilayer to diamondized film.

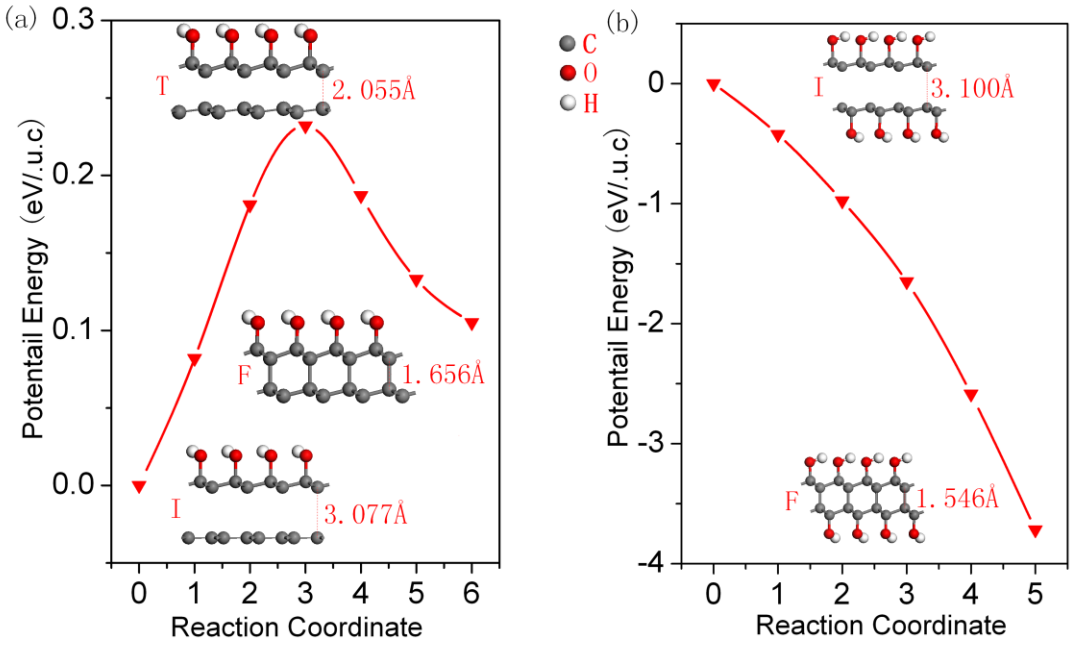

Fig. S2. Minimum energy path for transition processes (a) from single-side functionalized bilayer to diamondized film, (b) from double-side functionalized bilayer to diamondized film.

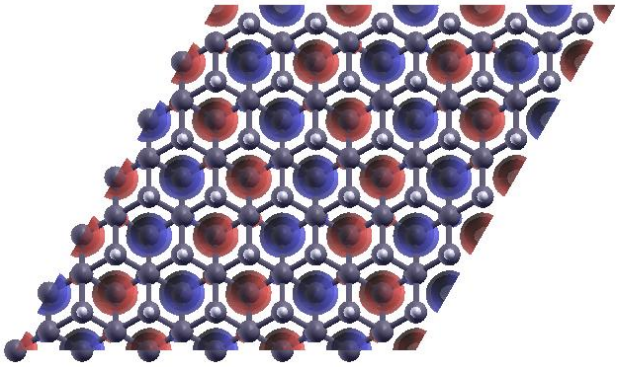

Fig. S3. Another AFM configuration with an energy 0.041 eV per unit cell higher than the FM ground state..

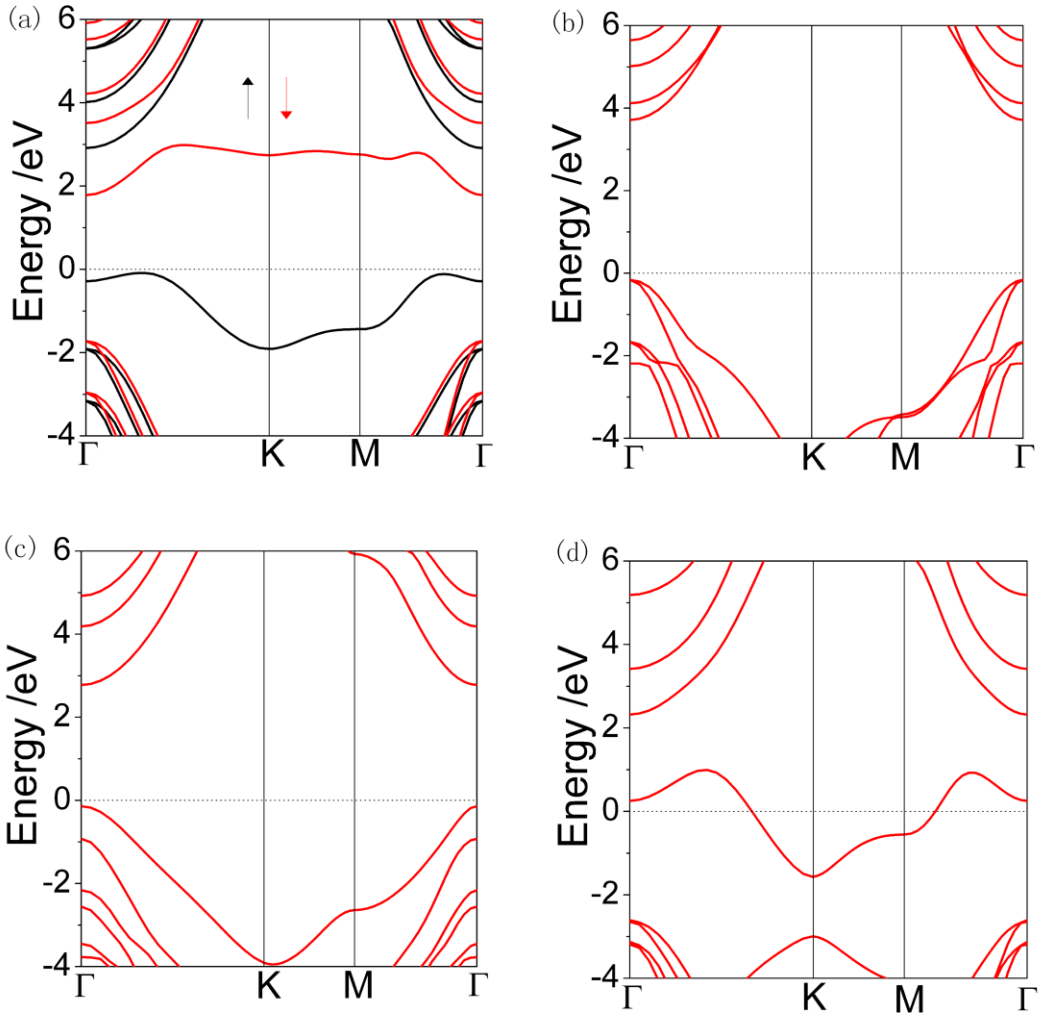

Fig. S4. HSE band structure of (a) H-C_2, (b) H-C_2-H, (c) H-C_2-OH, and (d) H-C-BN.

The band gap of *h*-BN layer is computed to evaluate the accuracy of our HSE procedure. The calculated band gap of *h*-BN layer is 5.69 eV, very close to the experiment value of 5.97 eV,[1] while PBE calculation predicts a band gap of 4.36 eV, underestimated by about 27% when compared to the experiment value. Three diamondol nanofilms such as H-C_2, H-C_2-H, and H-C_2-OH are computed for tests. For H-C_2, HSE band structure calculations predicts it a indrect semiconductor, with a band gap of 1.868 eV. For H-C_2-H and H-C_2-OH, HSE band structure calculations both predict that they are drect semiconductor, respectively, with a band gap of 3.875 eV and 2.917 eV. For H-C-BN, both PBE and HSE predict it a metal.

Notes and references

1. K. Watanabe, T. Taniguchi, H. Kanda, *Nat. Mater.*, 2004, 3, 404.