Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Confinement massless Dirac Fermions in graphene matrix induced by the B/N heteroatoms

Shansheng Yu,*[a,b] Weitao Zheng,[a] Zhimin Ao*[b,c] and Sean Li[b]

[a] Department of Materials Science, College of Materials Science and Engineering, Jilin University, Changchun, 130012, China.

[b] Department of Materials Science and Engineering, the University of New South Wales, 2052, Australia.

[c] School of Chemistry and Forensic Science, University of Technology, Sydney, 2007, Australia.

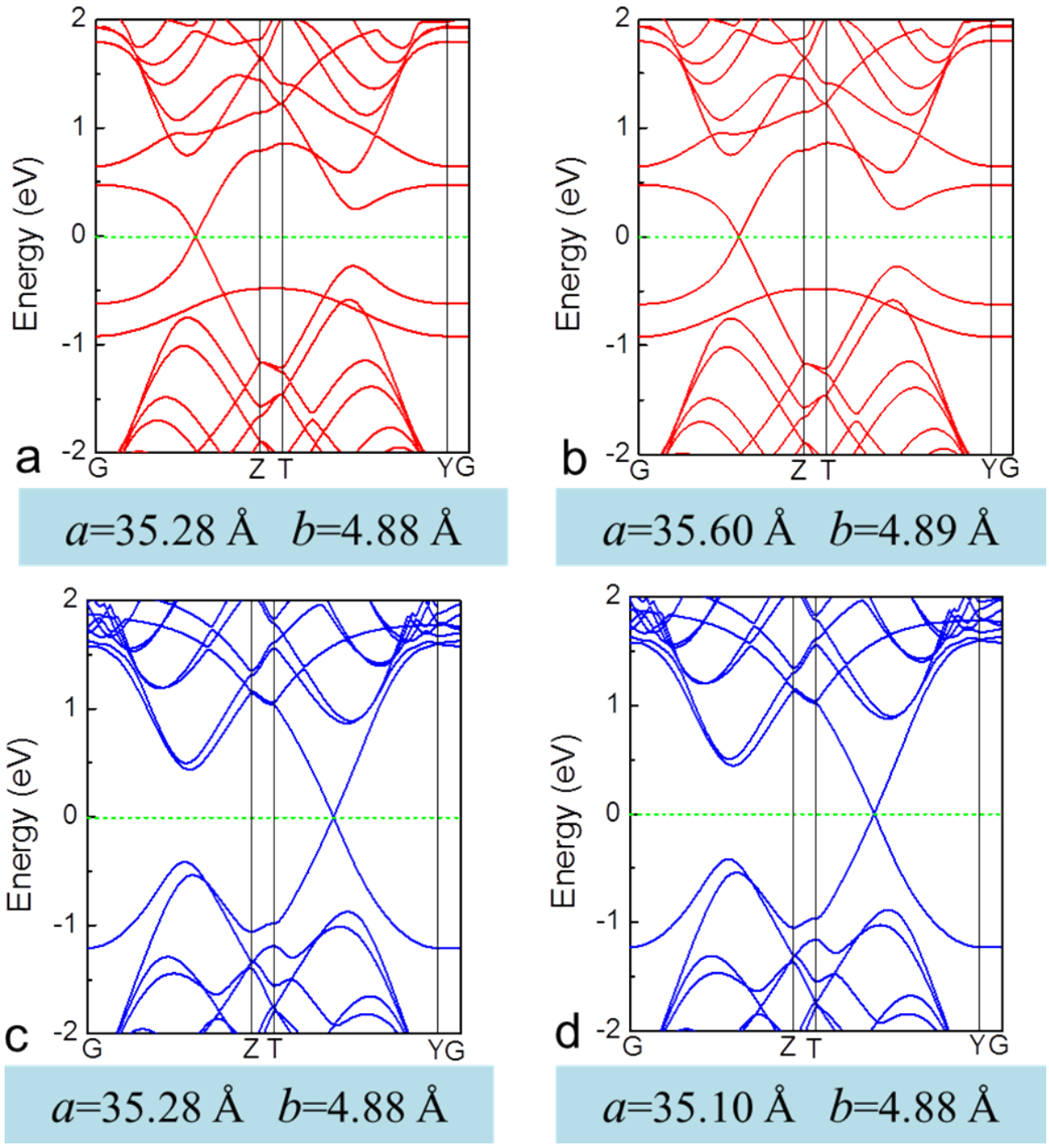
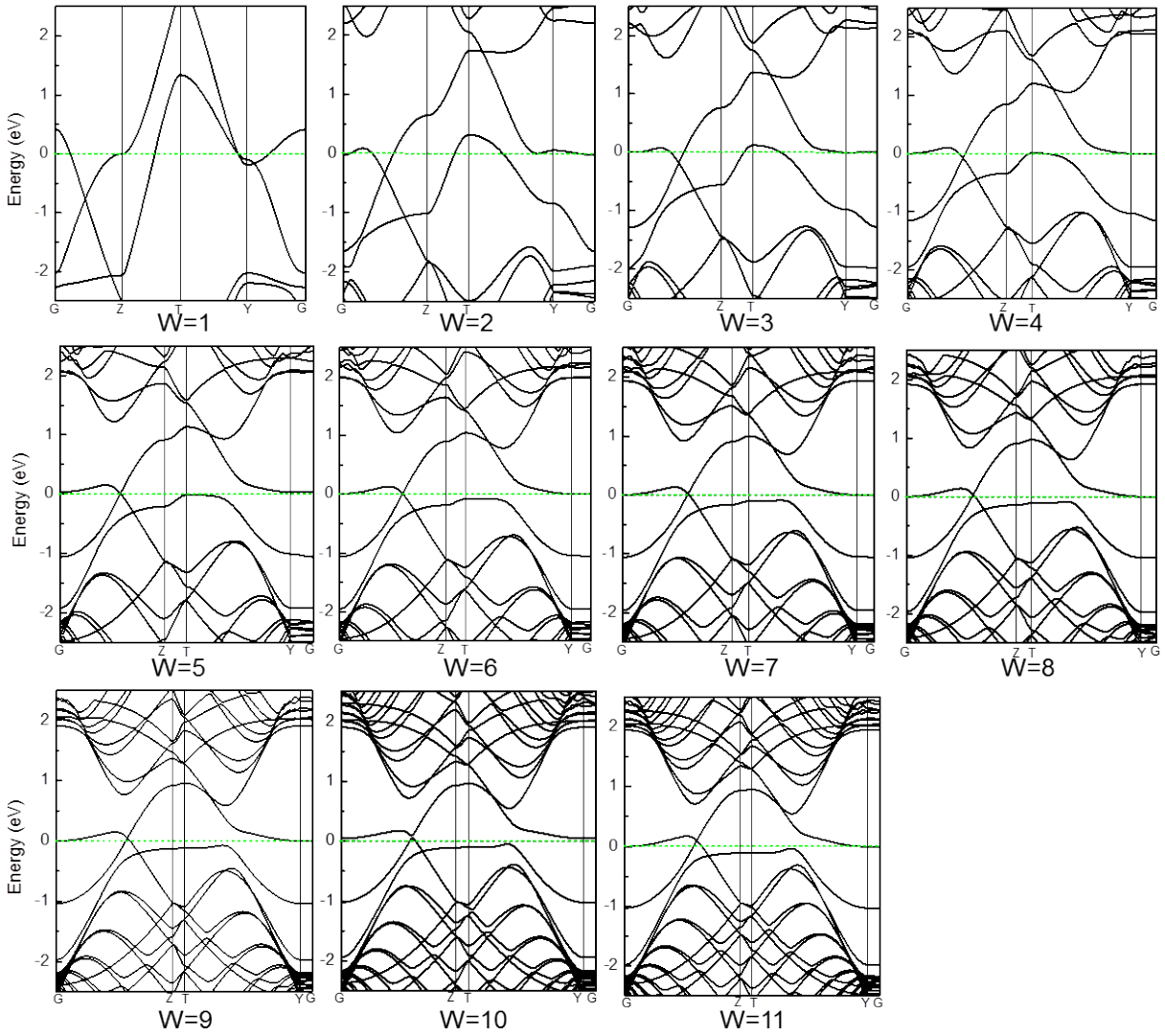


Fig. S1. Calculated band structures for B-B dimer case (a)(b) and N-N dimer case (c)(d) with W=8. (a) and (c) are results without relaxing cell lattices while (c) and (d) are results with relaxing cell lattices. a and b are parameters of unit cell along *x* and *y*.



(a)

Fig. S2a. The calculated band structures of graphene containing C-C dimer lines as a function of primitive cell width (W). The Fermi level of entire system is set as 0 eV.

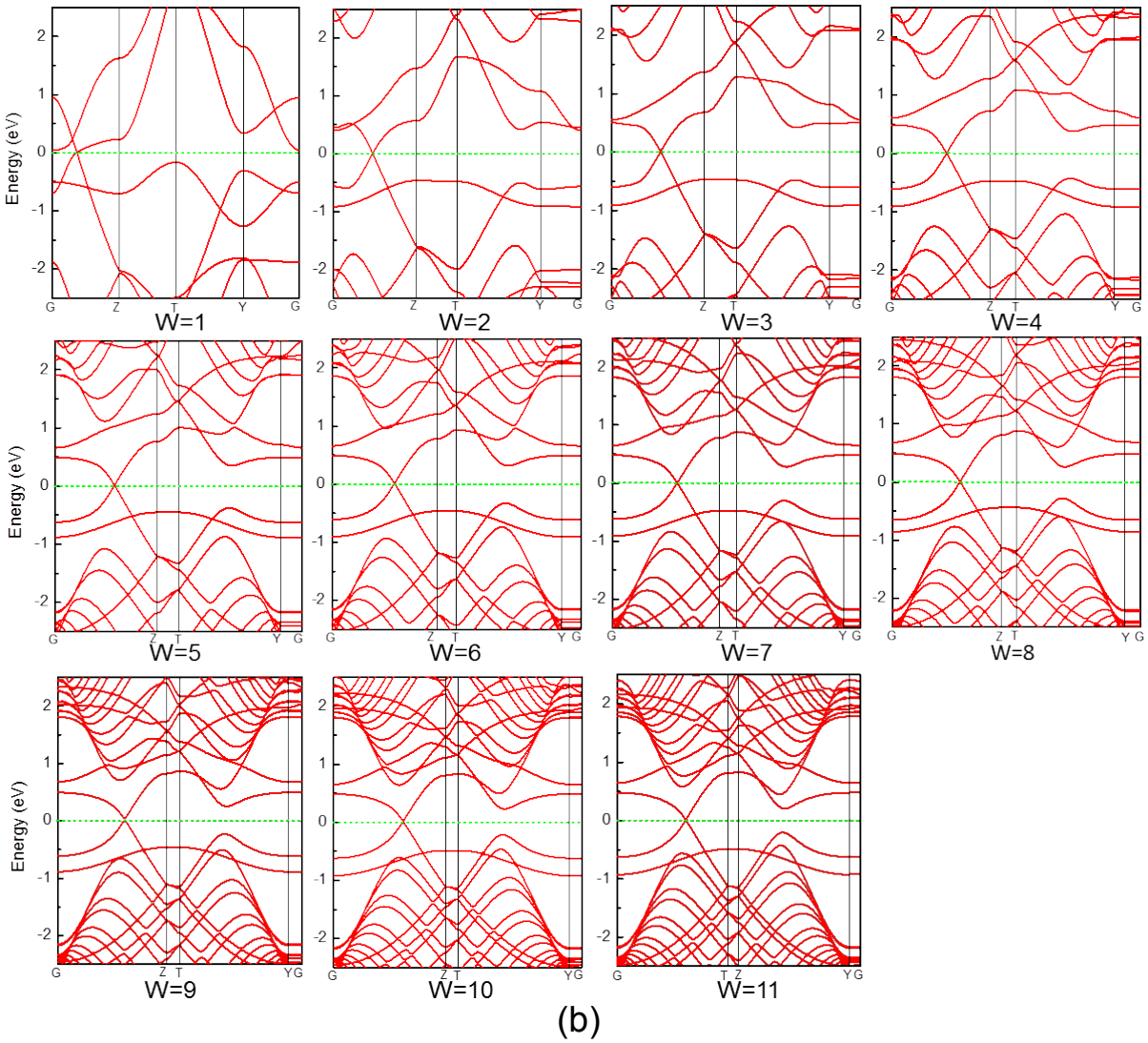


Fig. S2b. The calculated band structures of graphene containing B-B dimer lines as a function of primitive cell width (W). The Fermi level of entire system is set as 0 eV.

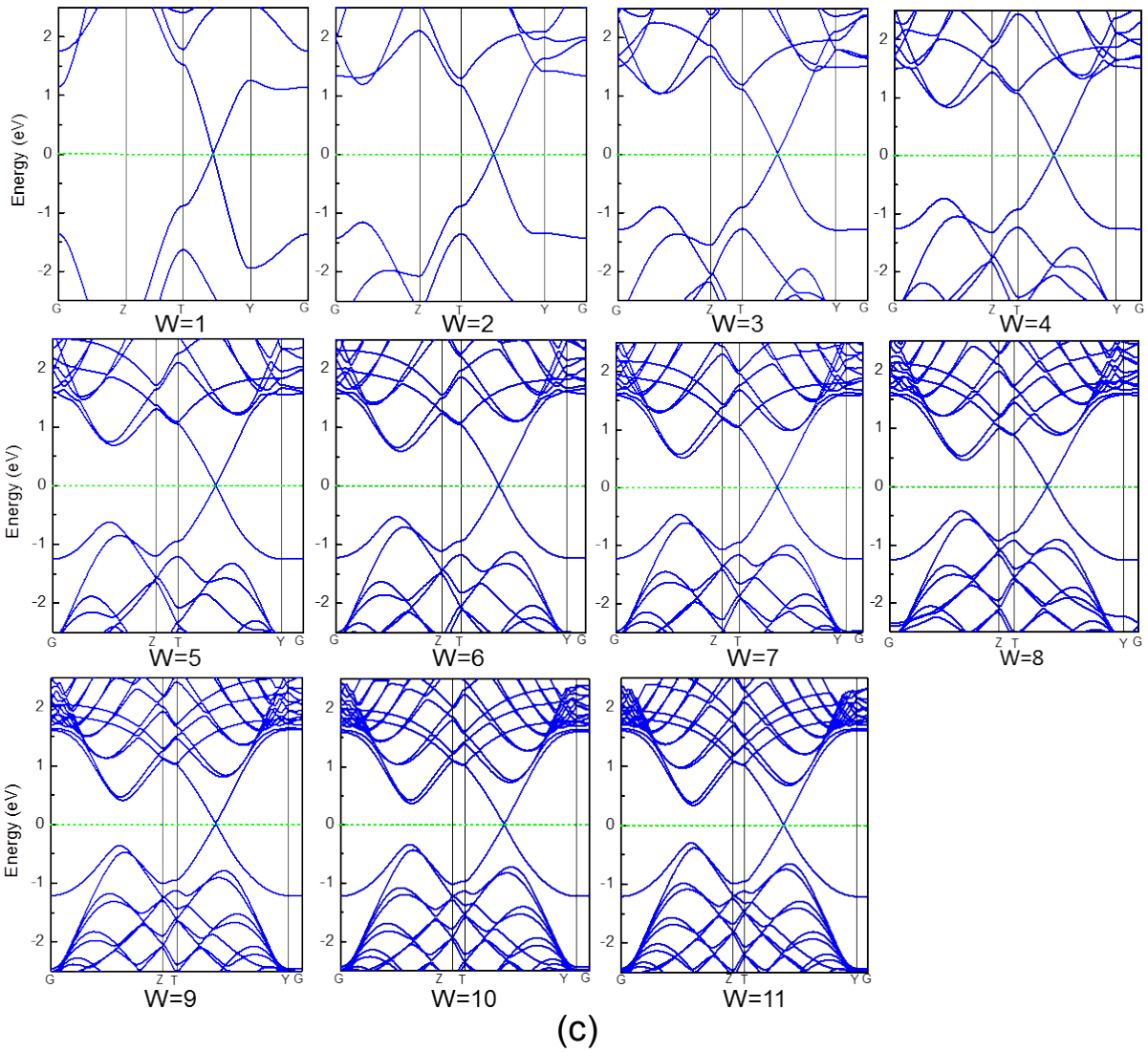


Fig. S2c. The calculated band structures of graphene containing N-N dimer lines as a function of primitive cell width (W). The Fermi level of entire system is set as 0 eV.

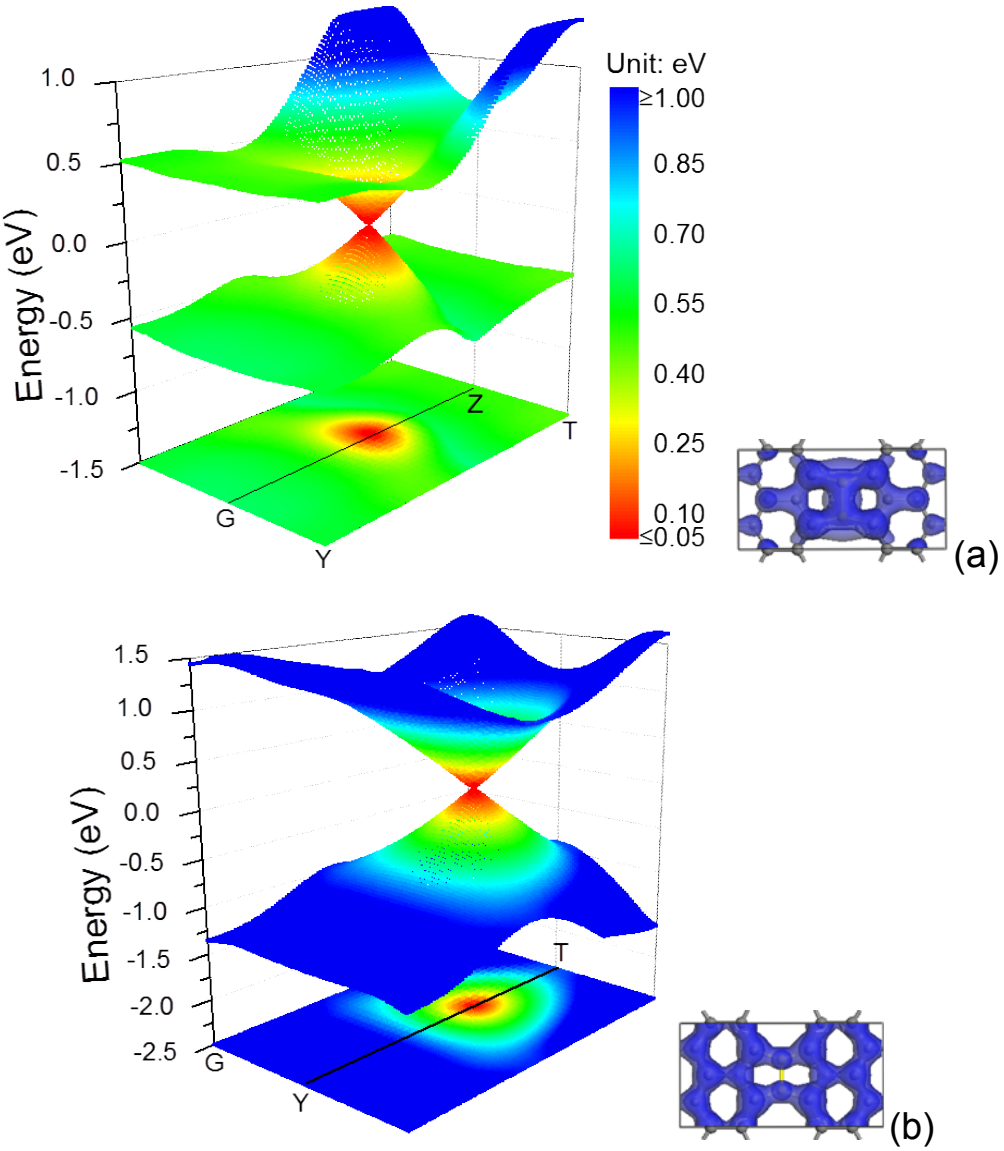


Fig. S3 3-D energy spectrum in a reciprocal space (left) and its corresponding electronic orbitals in a real space (right) for B-B (a)/N-N (b) dimer system with W=2: the first band dispersion above and below the Dirac point, and projection of first band below the Dirac point. Isosurface orbital contours are shown at the value of 0.015 electrons/a.u^3.

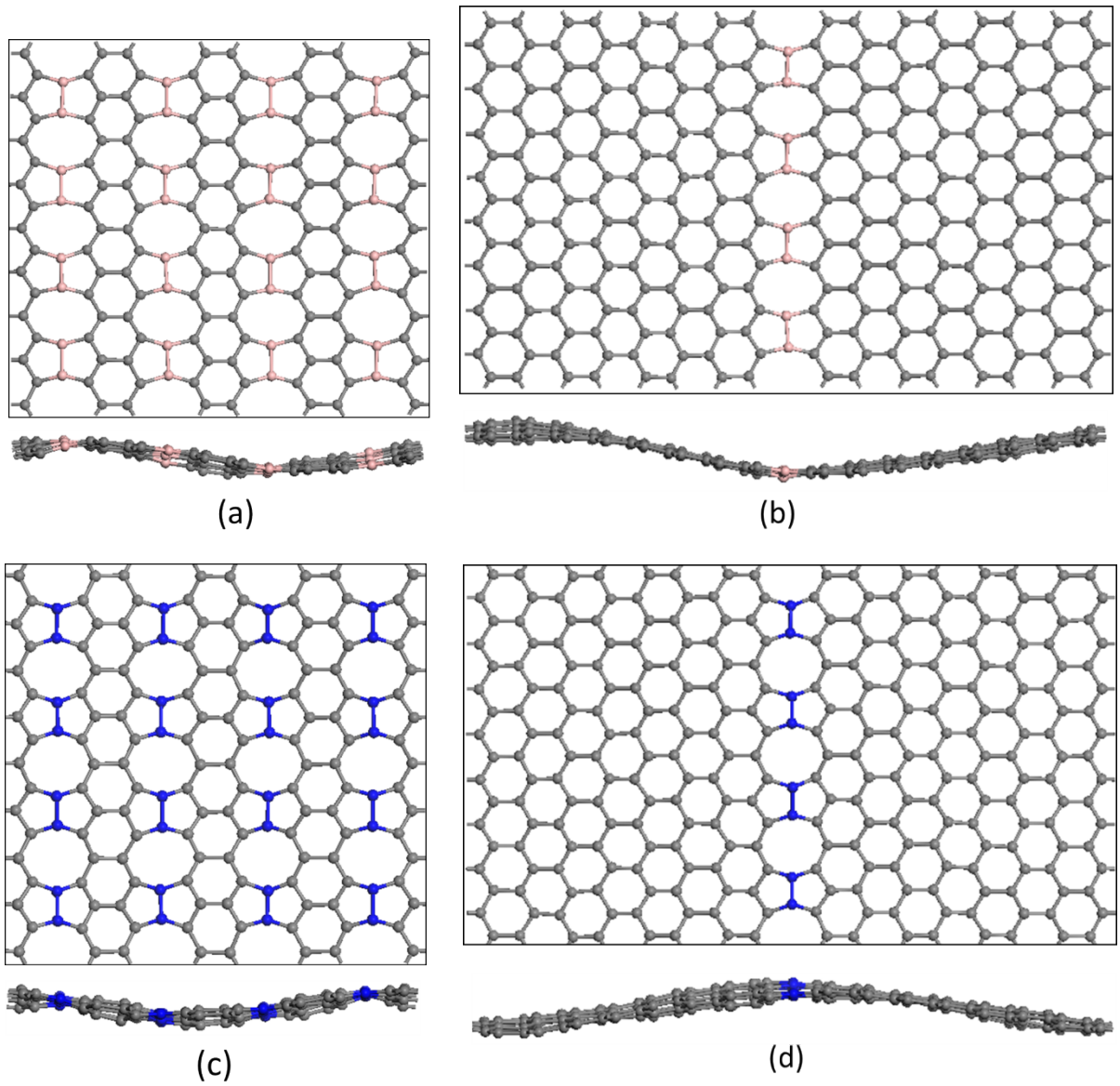


Fig. S3. Snapshots of B-B dimer system with W=1 (a) and 8 (b), and N-N dimer system with W=1 (c) and 8 (d) after a 3ps molecular dynamics simulation at 300K.

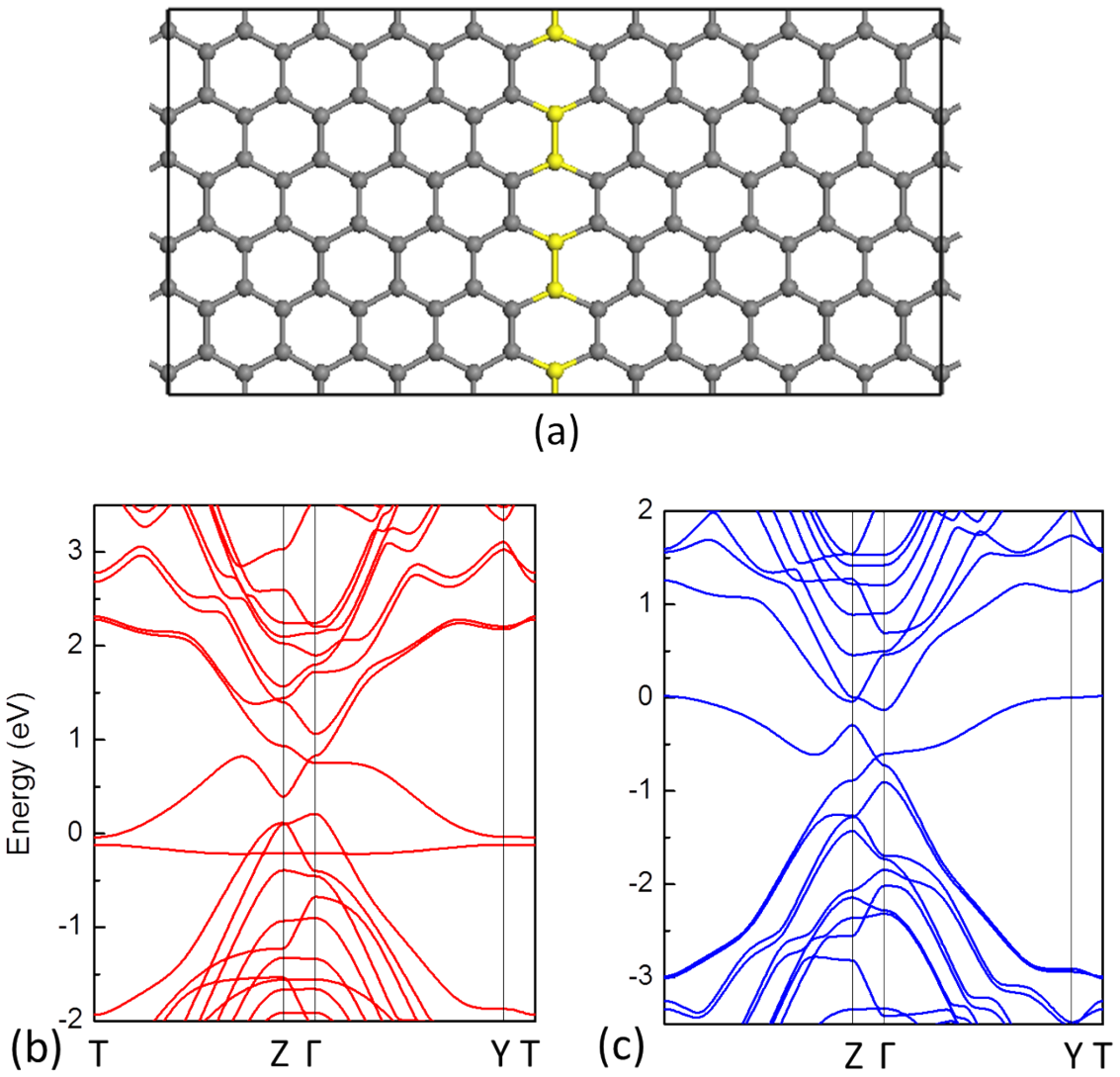


Fig. S4. (a) Structural model and schematic formation of an extended B-B/N-N dimer (yellow balls) line embedded in graphene. Both sides of the linear defects of B-B/N-N dimers are armchair edges. The band structures of (b) B-B dimer and (c) N-N dimer systems are exhibited.

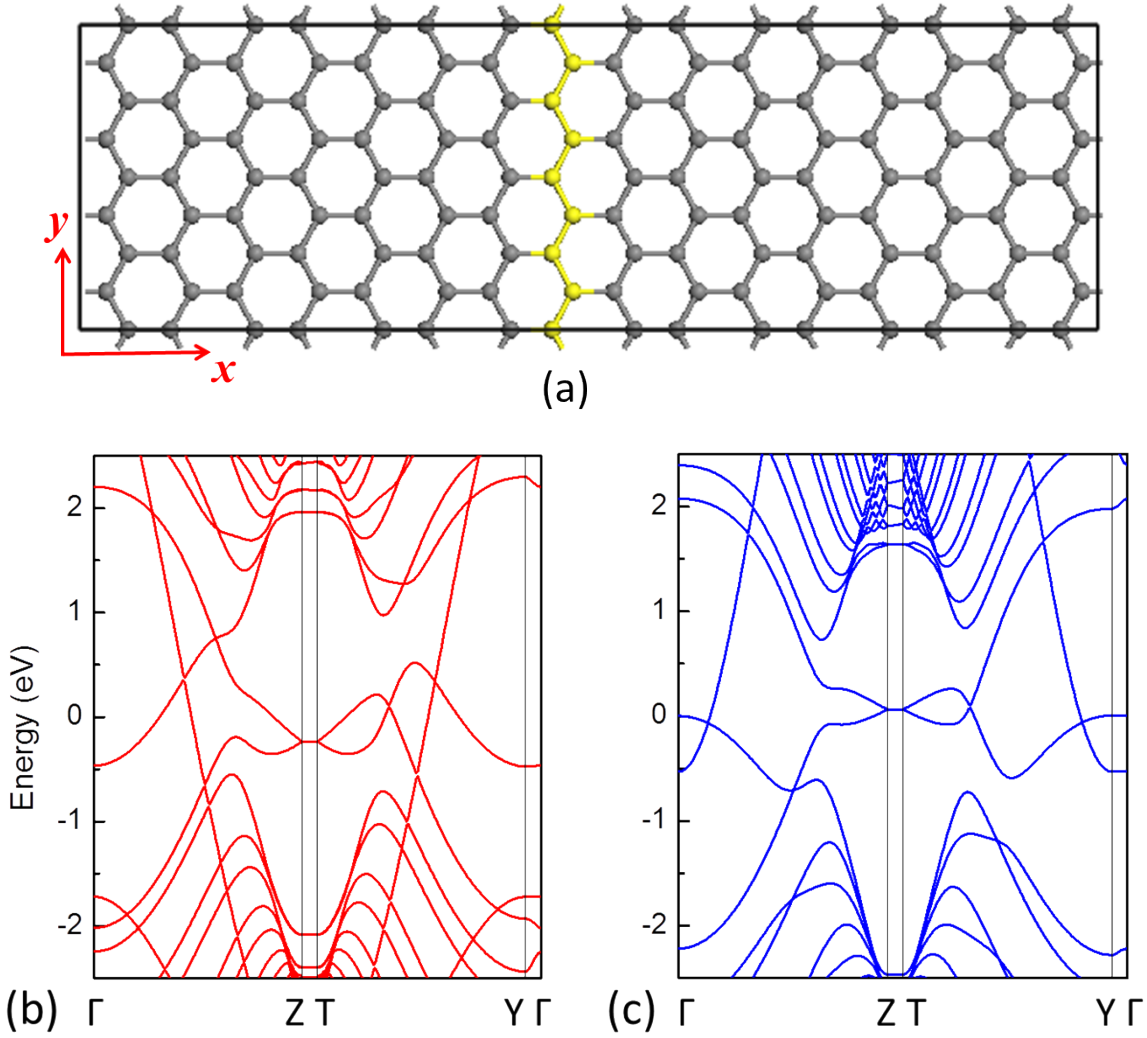


Fig. S5. (a) Structural model and schematic formation of a B/N atomic chain (yellow balls) embedded in graphene. Both sides of the B/N chain are zigzag edges. However, the two domains on the side of the B/N chain are translated by $1/3(a_1+a_2)$ relative to one another along the direction of *y*, contrary to dimer system in Fig. 1a which along the direction of *x*. The band structures of (b) B chain and (c) N chain systems are exhibited.