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

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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 \(y\).
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.