Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Benzene-like N_6 Rings in Be_2N_6 Monolayer: a Stable 2D Semiconductor with High Carrier Mobility

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Here are the supplementary figures and tables:

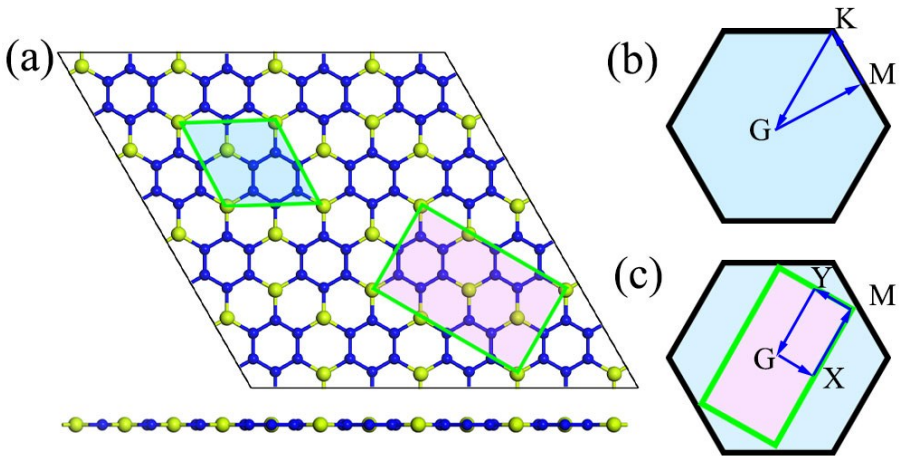

Figure S1. (a) Geometric structures of the unit cell (in blue) and tetragonal supercell (in pink) of Be_2N_6 monolayer. (b) Brillouin zones of the unit cell. The high-symmetry points are G(0,0,0), M(0.5,0,0), and K(-0.333,0.666,0) respectively. (c) Brillouin zones of the tetragonal supercell with four Be and twelve N atoms. The high-symmetry points are G(0,0,0), X(0.5,0,0), M(0.5,0.5,0), and Y(0,0.5,0) respectively.

Table S1. Optimized fractional positions of the unit cell for Be_2N_6 monolayer.

Be_2N_6

1.00000000000000

5.1475000380999996	0.0000000000000000	0.0000000000000000
-2.5737500190999998	4.4578657990000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

Direct

0.8333379651770656	0.1666620058229356	0.5000000000000000
0.1666620058229356	0.8333379651770656	0.5000000000000000
0.6528334042744390	0.3471665657255585	0.5000000000000000
0.1942972135943180	0.3471700871236578	0.5000000000000000
0.3471700871236578	0.1942972135943180	0.5000000000000000
0.3471665657255585	0.6528334042744390	0.5000000000000000
0.6528298828763397	0.8057028014056797	0.5000000000000000
0.8057028014056797	0.6528298828763397	0.5000000000000000

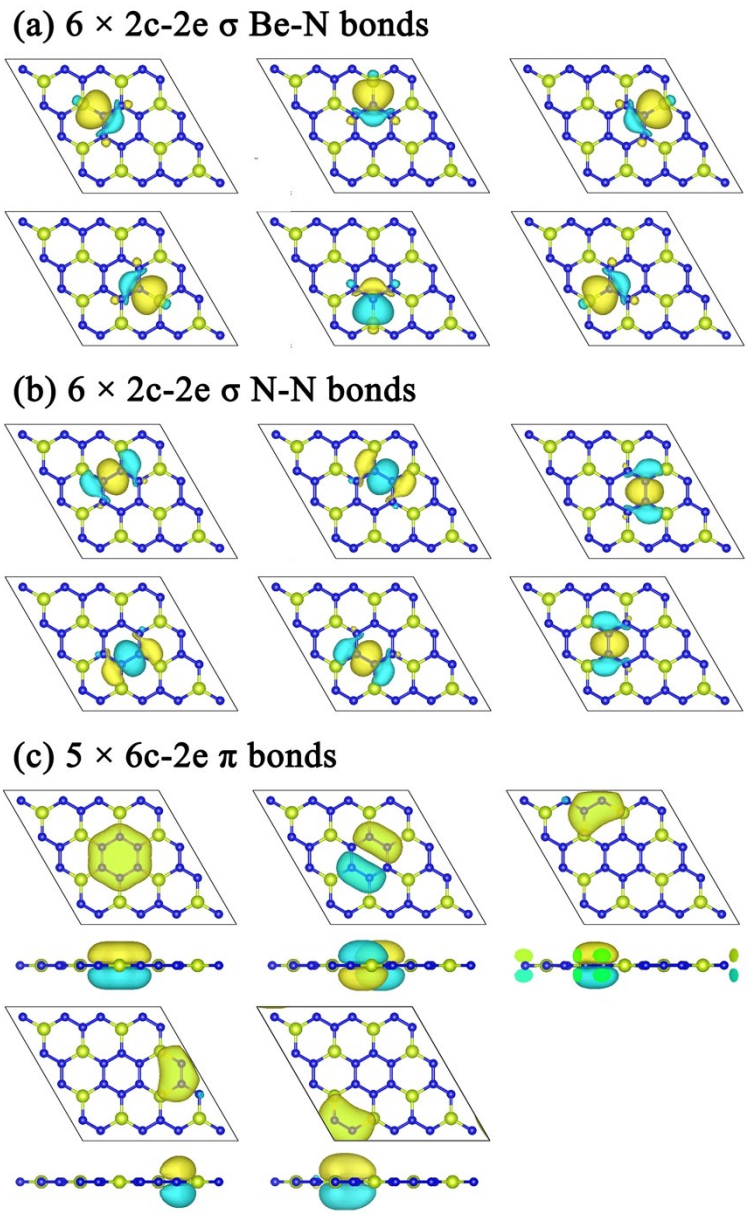

Figure S2. Chemical bonding pattern. Schematic of SSAdNDP chemical bonding pattern for a 2×2 supercell of Be_2N_6 monolayer, as marked as (a) six 2c-2e σ Be-N bonds, (b) six 2c-2e σ N-N bonds and (c) five novel 6c-2e π bonds, amount to 34 valence electrons in total. The iso-value is 0.02 e Å^{-3}.

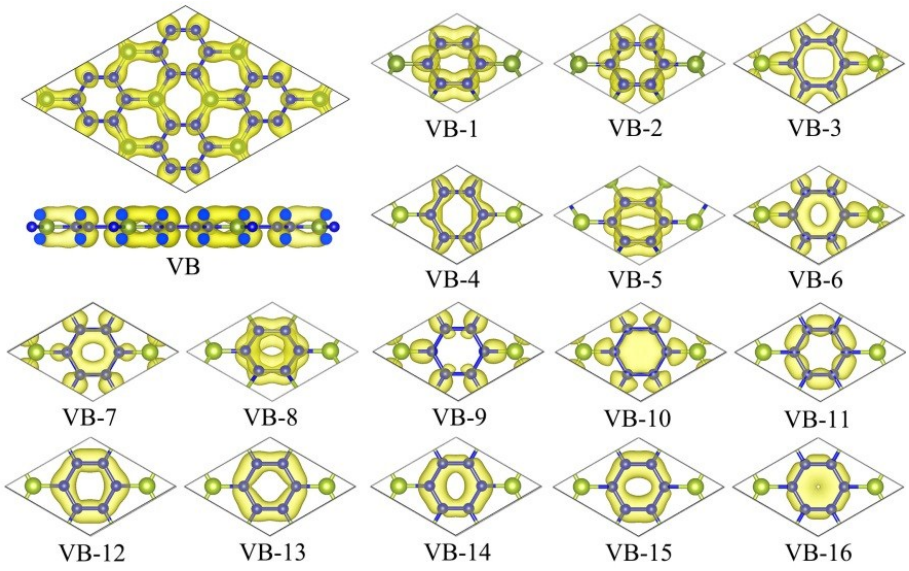

Figure S3 Charge densities of all the 17 occupied orbitals for Be_2N_6 monolayer, namely from valence band maximum to those in deeper energy. The iso-value is 0.005 e Å^{-3}.

An estimate of the 2D mobility can be then obtained using Takagi's formula.

$$\mu_{2D} = \frac{2e\hbar^3 C_{2D}}{3k_B T\left|m^*\right|^2 (E_l)^2}$$

where $\hbar$ is the reduced Planck constant, k_B is Boltzmann constant and T is the room temperature of 298 K. m^* is the effective mass in the transport directions. The x and y-axis represent along the armchair and zigzag directions, respectively. C_{2D} is the in-plane stiffness and can be determined by quadratic fitting of the total energy E with respect to the dilation $\Delta l/l_0$ as $(E - E_0)/S_0 = (C/2)(\Delta l/l_0)^2$ (Fig. S4), where S_0 is the equilibrium area. E_1 is the DP constant which denotes the shift of the band edge induced by the strain, as defined as $E_1 = \partial E_{edge}/\partial\varepsilon$ (Fig. S5). All of these quantities were computed at the HSE06 level.

A simple model gives the approximate relation between carrier mobility (μ) and relaxation time (τ). The relaxation time can be computed as:

$$\tau_{2D} = \frac{\mu_{2D} m^*}{e}$$

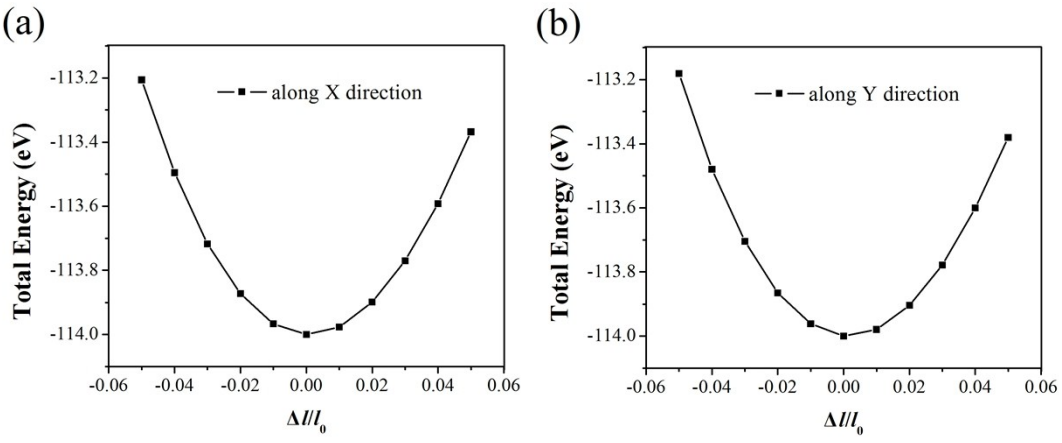

Figure S4. Strain–Total energy relations under the uniaxial strain of ±5 % along the (a) x and (b) y directions for Be_2N_6 monolayer. Δl and l_0 refer to the lattice dilation and lattice constant at equilibrium geometry.

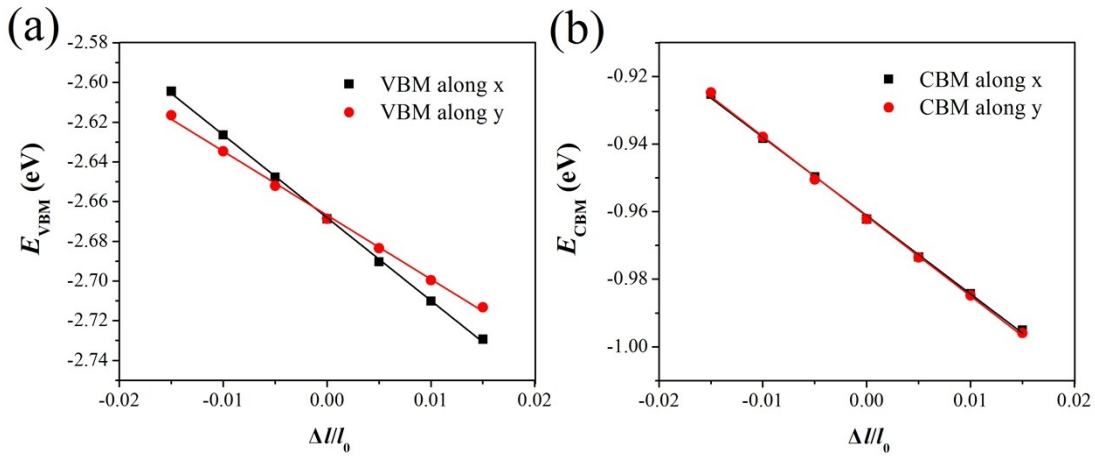

Figure S5. Shifts of (a) VBM and (b) CBM under the uniaxial strain of ±1.5 % along the *x* and *y* directions for Be_2N_6 monolayer. Δl and l_0 refer to the lattice dilation and lattice constant at equilibrium geometry.

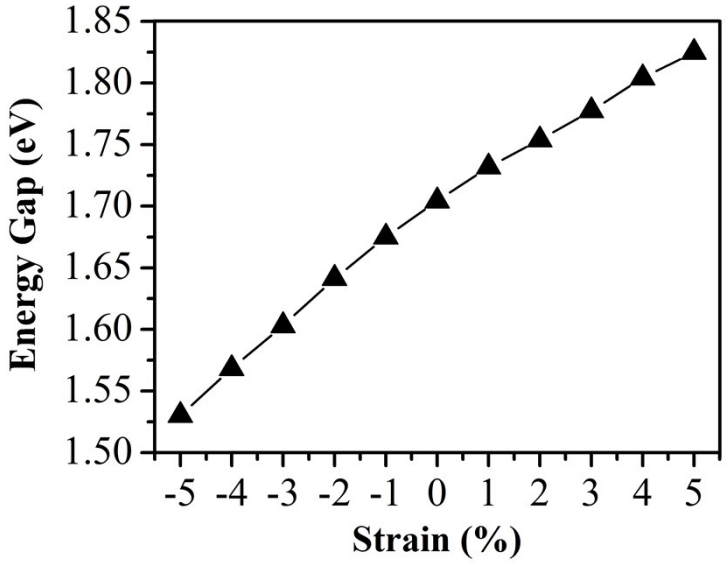

Figure S6. The modulation of the band gaps for Be_2N_6 monolayer via the external strains in the range of –5%~5% at the HSE06 level.

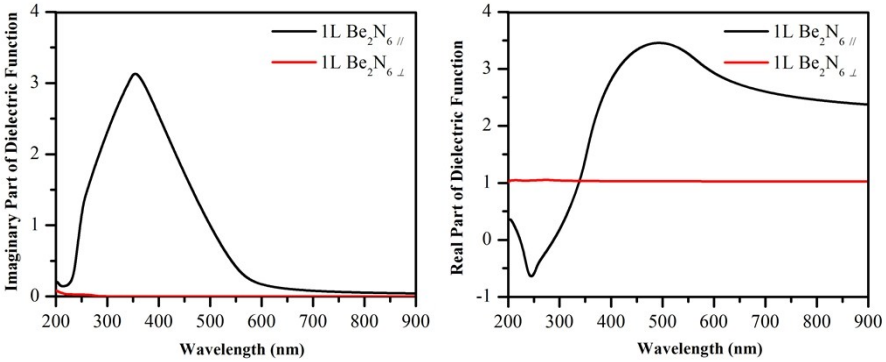

Figure S7. Imaginary and real part of dielectric function for Be_2N_6 monolayer in the directions of parallel (//) and perpendicular (⊥) to the incident light by using the tetrahedral method at the HSE06 level.

Geometric structures of isomers for Be_2N_6 bilayer. The binding energy per atom of the bilayer is defined by the equation of $E_{bin} = (2\times E_{1L} - E_{2L})/N$, in which E_{1L}, E_{2L}, and N represent the structural energy of the mono- and bi- layer and the number of atoms, respectively.

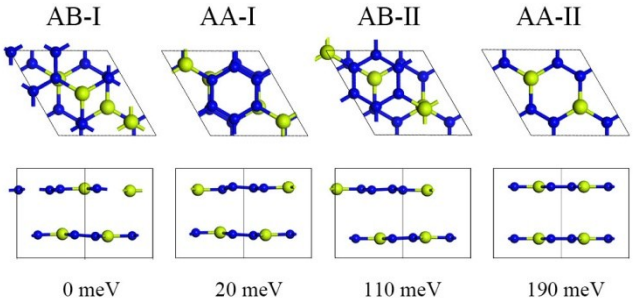

Figure S8. Top (upper) and side (bottom) view of the different configurations of Be_2N_6 bilayer, namely as AB–I, AA–I, AB–II, AA–II, respectively, marked with relative energy to the lowest-energy configuration.

Bader charge population analysis reveals that there is no considerable charge (< 1.0×10^{-4} |e|/cell) transfers between the layers in Be_2N_6 bilayer. This cannot induce any interlayer polarization, thus, Be_2N_6 bilayer would have a similar electronic property with the monolayer. Be_2N_6 bilayer has an HSE06 band gap of 1.63 eV (in Fig. S9), which is only 0.08 eV smaller than that of the monolayer (1.71 eV).

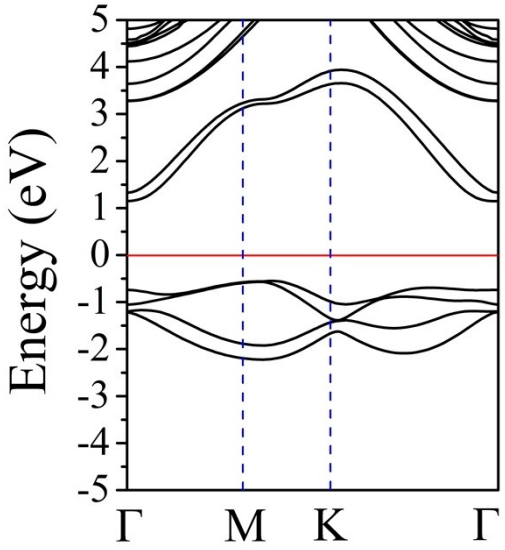

Figure S9. Band structure of Be_2N_6 bilayer computed at the HSE06 level.