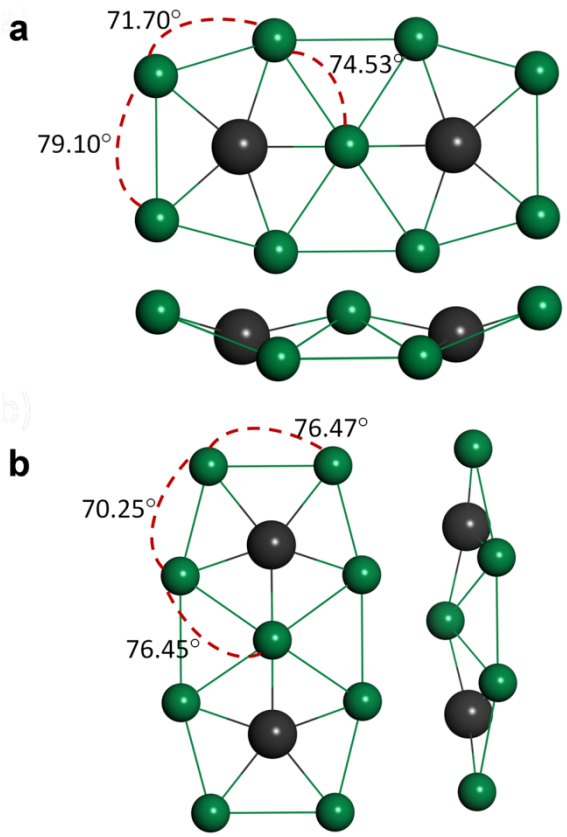
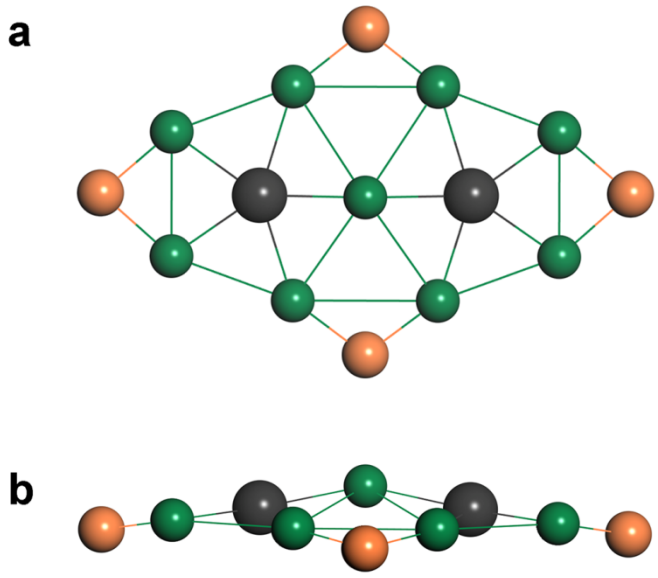
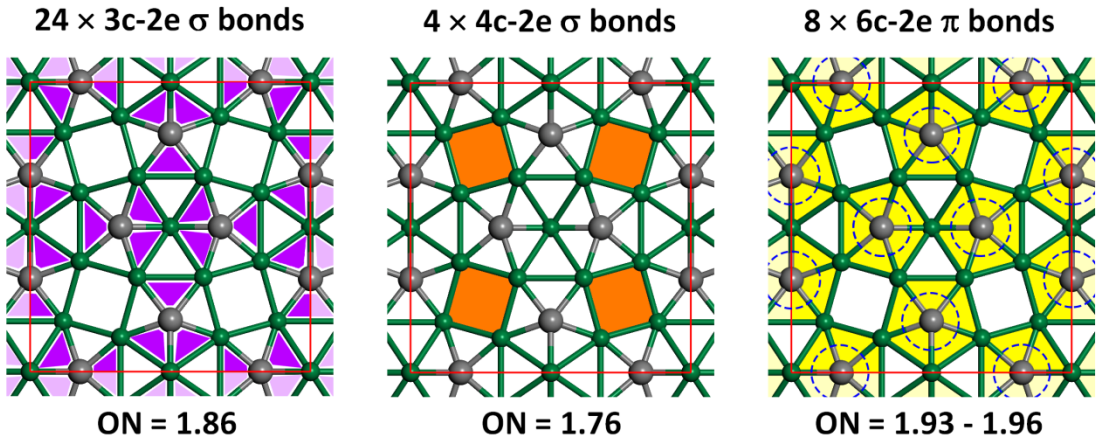


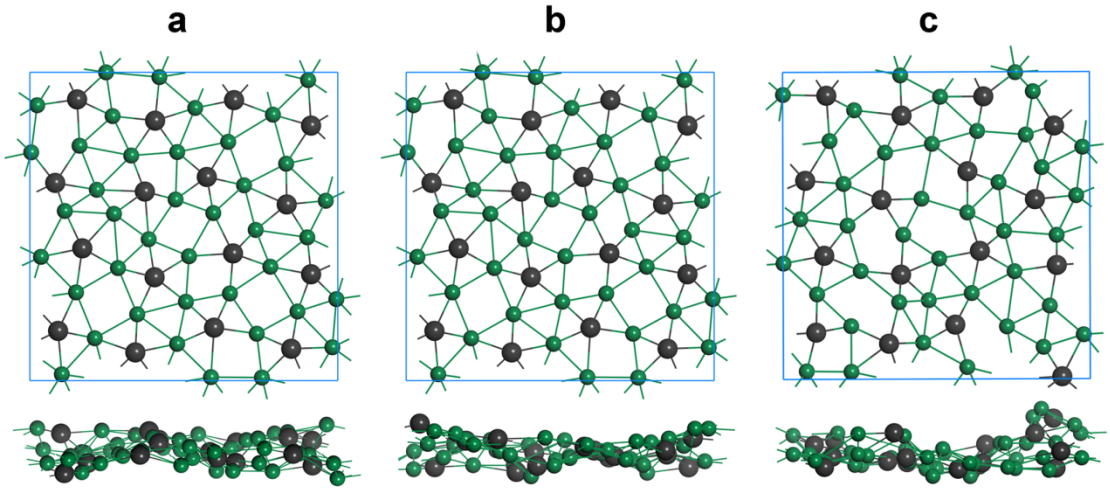

**Supplementary Figure 1: $Be_9C_2$ moieties.** Top and side views of $Be_9C_2$-I (a) and $Be_9C_2$-II (b) moieties in $Be_5C_2$ monolayer. The degrees of representative Be-C-Be angles are also given.



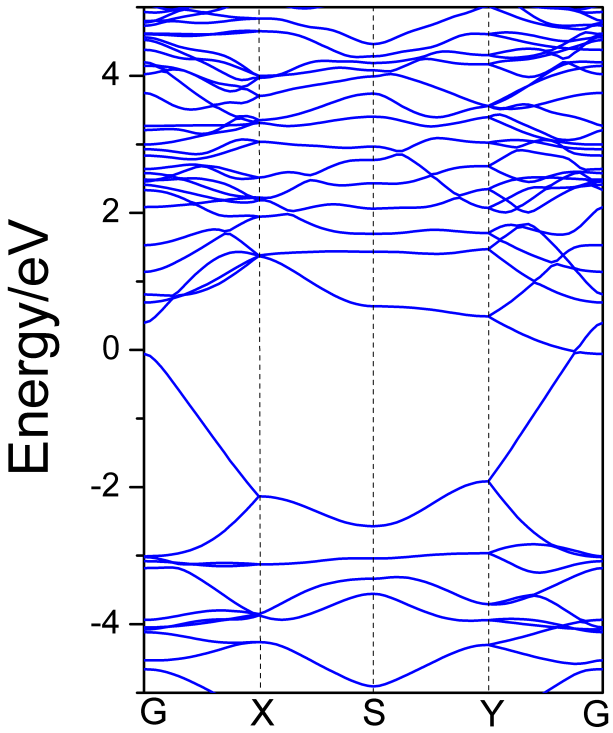

**Supplementary Figure 2: $Be_9C_2H_4$ molecule.** Top (a) and side (b) views of geometric structure of $Be_9C_2H_4$ molecule optimized at B3LYP/6-311+G*(d, p) level of theory. Yellow balls represent H atoms.




**Supplementary Figure 3: Chemical bonding pattern.** Schematic of SSAdNDP chemical bonding pattern for a unit cell of $Be_5C_2$ monolayer.




**Supplementary Figure 4: Molecular dynamics simulations.** A snapshot of the equilibrium structure of $Be_5C_2$ monolayer at (a) 1000 K, (b) 1500 K, and (c) 2000 K, respectively, at the end of 10 ps first-principles molecular dynamics simulation.




**Supplementary Figure 5: Electronic properties of $Be_5C_2$ monolayer.** Band structure of $Be_5C_2$ monolayer computed using HSE06 functional.

**Supplementary Table 1:** Optimized coordinates of the unit cell for $Be_2C_5$ monolayer.

$Be_2C_5$

1.0000000000000000

| | | |
|---|---|---|
| 8.9200000000000000 | 0.0000000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 9.2060000000000000 | 0.0000000000000000 |
| 0.0000000000000000 | 0.0000000000000000 | 15.0000000000000000 |

| | | | |
|---|---|---|---|
| Be | 0.67587 | 0.88103 | 0.5114 |
| Be | 0.12065 | 0.17457 | 0.46288 |
| Be | 0.32413 | 0.11897 | 0.5114 |
| Be | 0.87935 | 0.82543 | 0.46288 |
| Be | 0.82413 | 0.38103 | 0.4886 |
| Be | 0.37935 | 0.67457 | 0.53712 |
| Be | 0.17587 | 0.61897 | 0.4886 |
| Be | 0.62065 | 0.32543 | 0.53712 |
| Be | 0.82413 | 0.61897 | 0.4886 |
| Be | 0.37935 | 0.32543 | 0.53712 |
| Be | 0.17587 | 0.38103 | 0.4886 |
| Be | 0.62065 | 0.67457 | 0.53712 |
| Be | 0.67587 | 0.11897 | 0.5114 |
| Be | 0.12065 | 0.82543 | 0.46288 |
| Be | 0.32413 | 0.88103 | 0.5114 |
| Be | 0.87935 | 0.17457 | 0.46288 |
| Be | 0 | 0 | 0.5091 |
| Be | 0.5 | 0.5 | 0.4909 |
| Be | 0.5 | 0 | 0.57173 |
| Be | 0 | 0.5 | 0.42827 |
| C | 0.5 | 0.82226 | 0.54597 |
| C | 0.5 | 0.17774 | 0.54597 |
| C | 0 | 0.32226 | 0.45403 |
| C | 0 | 0.67774 | 0.45403 |
| C | 0.68188 | 0.5 | 0.51428 |
| C | 0.31812 | 0.5 | 0.51428 |
| C | 0.81812 | 0 | 0.48572 |
| C | 0.18188 | 0 | 0.48572 |