

Supporting Information (SI)

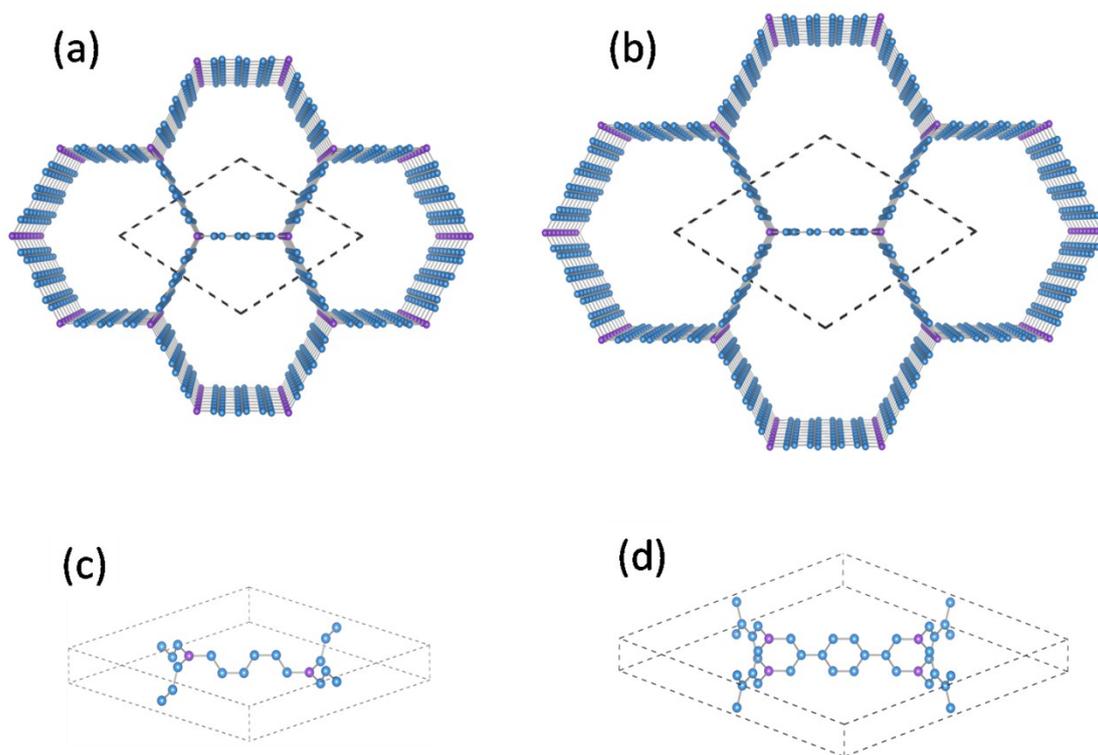


FIG S1. Atomic structures of (a) CHC-3 and (b) CHC-4. Legends are the same as in Fig. 1.

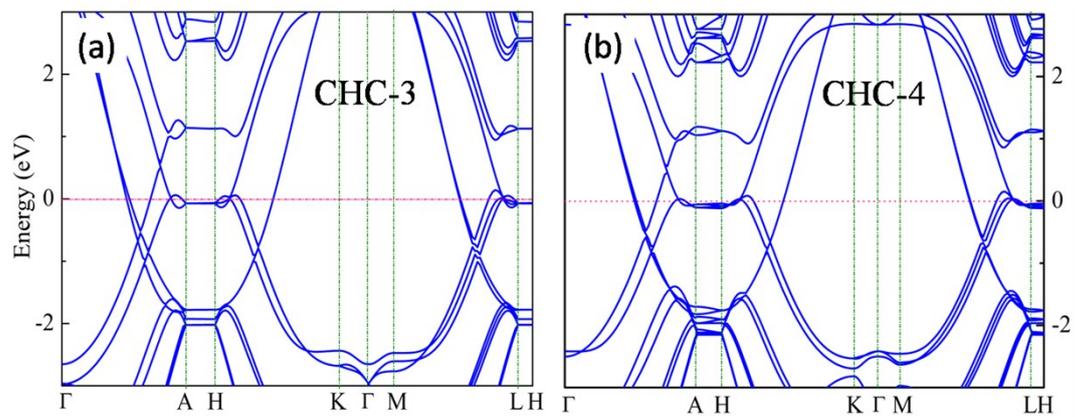


FIG S2. DFT band structures of (a) CHC-3 and (b) CHC-4.

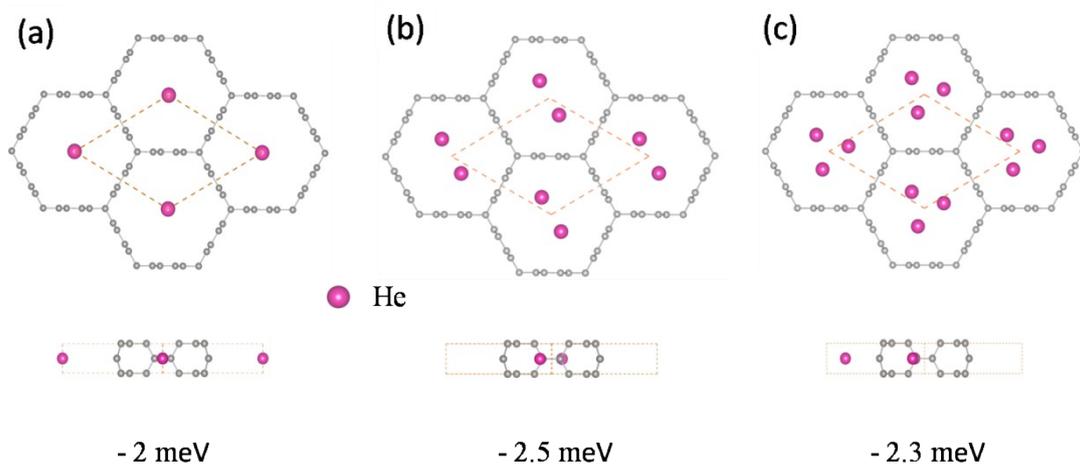


FIG S3. Top and side views of (a) one, (b) two, (c) three He adsorption in the $1 \times 1 \times 1$ primitive cell of CHC-2. Average adsorption energy E_N/N has been indicated. Legends are the same as in Fig. 6.

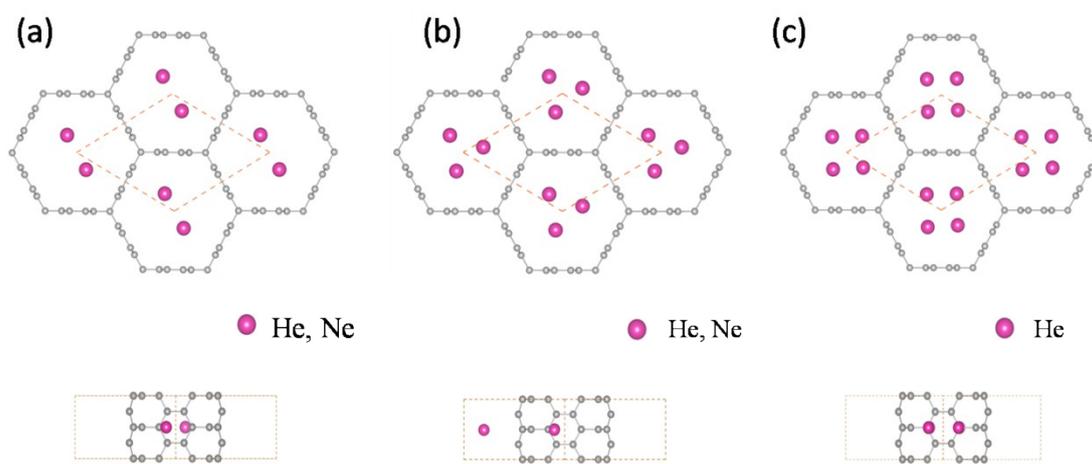


FIG S4. Top and side views of (a) two, (b) three, (c) four inert gas atoms adsorption in the $1 \times 1 \times 2$ supercell of CHC-2. Legends are the same as in Fig. 6.

Table S1. Consecutive adsorption energy δE_C for He loading of CHC-4. All energies are given in meV/He. ρ is the corresponding adsorption density in atomic weight percent.

| #adsorbent | δE_C | ρ (wt%) |
|------------|--------------|--------------|
| 16 | -16 | 17.0 |
| 17 | -12 | 17.9 |
| 18 | -10 | 18.8 |
| 19 | -7 | 19.6 |
| 20 | +10 | 20.4 |