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


# Supporting Information to

## Boron-rich Hybrid BCN Nanoribbons as Highly Ambient Uptake of Toxic Gases; $H_2S$, HF, $NH_3$, CO, $CO_2$

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# Contents

**Table S1:** The length of C-B, C-N, B-N and B-B bonds in 6-ACBNNR with 33%-C, 8-ZCBNNR with 25%-C, B-rich 6- ACBNNR with 33%-C and B-rich 8-ZCBNNR with 25%-C. B-B bond is created due to B atoms replacing C atoms in boron-rich nanoribbons.

| bond / nanoribbon | C-B | C-N | B-N | B-B |
|---|---|---|---|---|
| 6-ACBNNR with 33%-C | 1.41 Å | 1.39 Å | 1.44 Å | - |
| 8-ZCBNNR with 25%-C | 1.48 Å | 1.42 Å | 1.44 Å | - |
| B-rich 6- ACBNNR with 33%-C | 1.49 Å | 1.39 Å | 1.44 Å | 1.58 Å |
| B-rich 8-ZCBNNR with 25%-C | 1.48 Å | 1.42 Å | 1.44 Å | 1.67 Å |

**Table S2:** Fermi energy ($E_F$), energy band gap ($E_g$) and electrical conductivity of 6-ACBNNR with 33%-C, 8-ZCBNNR with 25%-C, B-rich 6-ACBNNR with 33%-C and B-rich 8-ZCBNNR with 25%-C before gas molecule adsorption.

| substrate | $\boldsymbol{E_F(eV)}$ | $\boldsymbol{E_g(eV)}$ | electrical conductivity |
|---|---|---|---|
| 6-ACBNNR with 33%-C | -3.318 | 0.761 | semiconductor |
| 8-ZCBNNR with 25%-C | -3.303 | 0.901 | semiconductor |
| B-rich 6- ACBNNR with 33%-C | -3.600 | 0 | metal |
| B-rich 8-ZCBNNR with 25%-C | -3.409 | 0 | metal |

**Table S3:** CO molecule adsorbed on 6-ACBNNR with 33%-C, 8-ZCBNNR with 25%-C, B-rich 6-ACBNNR with 33%-C and B-rich 8-ZCBNNR with 25%-C: the bond length of gas molecule (L), adsorption distance of nearest-neighbor atoms between the gas molecule and substrate (D), the angle of gas molecule ($\alpha$), charge transfer between gas molecule and substrate ($\Delta Q$), the sign "-" means that the molecule is the acceptor of the charge and the sign "+" means the molecule is the donor of the charge, and adsorption energy ($E_{ads}$). The words "before" and "after" express the characteristics of the gas molecule before and after gas molecule adsorption, respectively.

| **CO molecule adsorption** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **substrate** | **L (Å)** | | **D (Å)** | | **$\alpha$ (°)** | | **$\Delta Q$ ($e$)** | **$E_{ads}$ ($eV$)** | **Type of adsorption** |
| | **before** | **after** | **before** | **after** | **before** | **after** | | | |
| 6-ACBNNR with 33%-C | 1.145 | 1.144 | 2.455 | 2.976 | - | - | -0.010 | -1.483 | physisorption |
| 8-ZCBNNR with 25%-C | | 1.147 | 2.128 | 3.040 | | - | -0.019 | -0.845 | physisorption |
| B-rich 6-ACBNNR with 33%-C | | 1.160 | 2.000 | 1.616 | | - | +0.124 | -2.275 | chemisorption |
| B-rich 8-ZCBNNR with 25%-C | | 1.153 | 2.000 | 1.599 | | - | +0.190 | -1.294 | chemisorption |

**Table S4:** Fermi energy ($E_F$), energy band gap ($E_g$), structural deformation (Δ) and electrical conductivity of 6-ACBNNR with 33%-C, 8-ZCBNNR with 25%-C, B-rich 6-ACBNNR with 33%-C and B-rich 8-ZCBNNR with 25%-C after CO molecule adsorption.

| **system** | **$E_F(eV)$** | **$E_g(eV)$** | Δ(Å) | **electrical conductivity** |
|---|---|---|---|---|
| 6-ACBNNR with 33%-C + CO | -3.62 | 0.875 | 1.559 | semiconductor |
| 8-ZCBNNR with 25%-C + CO | -3.33 | 0.866 | 0.737 | semiconductor |
| B-rich 6-ACBNNR with 33%-C + CO | -3.281 | 0 | 1.588 | metal |
| B-rich 8-ZCBNNR with 25%-C + CO | -2.950 | 0 | 0.839 | metal |

**Table S5:** $CO_2$ molecule adsorbed on 6-ACBNNR with 33%-C, 8-ZCBNNR with 25%-C, B-rich 6-ACBNNR with 33%-C and B-rich 8-ZCBNNR with 25%-C: the bond length of gas molecule (L), adsorption distance of nearest-neighbor atoms between the gas molecule and substrate (D), the angle of gas molecule ($\alpha$), charge transfer between gas molecule and substrate ($\Delta Q$), the sign "-" means that the molecule is the acceptor of the charge and the sign "+" means the molecule is the donor of the charge, and adsorption energy ($E_{ads}$). The words "before" and "after" express the characteristics of the gas molecule before and after gas molecule adsorption, respectively.

| **$CO_2$ molecule adsorption** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **substrate** | **L (Å)** | | **D (Å)** | | **$\alpha$ (°)** | | **$\Delta Q$ ($e$)** | **$E_{ads}$ ($eV$)** | **Type of adsorption** |
| | **before** | **after** | **before** | **after** | **before** | **after** | | | |
| 6-ACBNNR with 33%-C | C-O1 =1.178 | C-O1 =1.182<br>C-O2 =1.178 | 2.016 | 2.982 | 180 | 178.703 | -0.008 | -1.602 | physisorption |
| 8-ZCBNNR with 25%-C | C-O2 =1.178 | C-O1 =1.181<br>C-O2 =1.181 | 2.128 | 3.060 | | 178.571 | -0.013 | -0.998 | physisorption |
| B-rich 6-ACBNNR with 33%-C | | C-O1 =1.180<br>C-O2 =1.179 | 2.022 | 2.968 | | 179.846 | +0.013 | -1.926 | physisorption |
| B-rich 8-ZCBNNR with 25%-C | | C-O1 =1.180<br>C-O2 =1.181 | 2.027 | 3.001 | | 178.194 | -0.008 | -1.079 | physisorption |

**Table S6:** Fermi energy ($E_F$), energy band gap ($E_g$), structural deformation (Δ) and electrical conductivity of 6-ACBNNR with 33%-C, 8-ZCBNNR with 25%-C, B-rich 6-ACBNNR with 33%-C and B-rich 8-ZCBNNR with 25%-C after $CO_2$ molecule adsorption.

| **system** | $\boldsymbol{E_F(eV)}$ | $\boldsymbol{E_g(eV)}$ | Δ(Å) | **electrical conductivity** |
|---|---|---|---|---|
| 6-ACBNNR with 33%-C + $CO_2$ | -3.295 | 0.875 | 1.549 | semiconductor |
| 8-ZCBNNR with 25%-C + $CO_2$ | -3.270 | 0.884 | 0.730 | semiconductor |
| B-rich 6-ACBNNR with 33%-C + $CO_2$ | -3.687 | 0 | 1.584 | metal |
| B-rich 8-ZCBNNR with 25%-C + $CO_2$ | -3.469 | 0 | 0.793 | metal |

**Table S7:** $H_2S$ molecule adsorbed on 6-ACBNNR with 33%-C, 8-ZCBNNR with 25%-C, B-rich 6-ACBNNR with 33%-C and B-rich 8-ZCBNNR with 25%-C: the bond length of gas molecule (L), adsorption distance of nearest-neighbor atoms between the gas molecule and substrate (D), the angle of gas molecule ($\alpha$), charge transfer between gas molecule and substrate ($\Delta Q$), the sign "-" means that the molecule is the acceptor of the charge and the sign "+" means the molecule is the donor of the charge, and adsorption energy ($E_{ads}$). The words "before" and "after" express the characteristics of the gas molecule before and after gas molecule adsorption, respectively.

**$H_2S$ molecule adsorption**

| **substrate** | **L (Å)** | | **D (Å)** | | **$\alpha$ (°)** | | **$\Delta Q$ ($e$)** | **$E_{ads}$ ($eV$)** | **Type of adsorption** |
|---|---|---|---|---|---|---|---|---|---|
| | **before** | **after** | **before** | **after** | **before** | **after** | | | |
| 6-ACBNNR with 33%-C | S-H1 =1.371 | S-H1 =1.374<br>S-H2 =1.371 | 3.635 | 2.930 | | 91.543 | -0.019 | -1.510 | physisorption |
| 8-ZCBNNR with 25%-C | S-H2 =1.371 | S-H1 =1.371<br>S-H2 =1.370 | 2.128 | 3.239 | 92.033 | 91.267 | -0.009 | -0.863 | physisorption |
| B-rich 6-ACBNNR with 33%-C | | S-H1 =1.372<br>S-H2 =1.375 | 3.015 | 2.991 | | 91.925 | +0.076 | -1.972 | physisorption |
| B-rich 8-ZCBNNR with 25%-C | | S-H1 =1.372<br>S-H2 =1.372 | 2.000 | 3.036 | | 92.114 | +0.069 | -0.992 | physisorption |

**Table S8:** Fermi energy ($E_F$), energy band gap ($E_g$), structural deformation (Δ) and electrical conductivity of 6-ACBNNR with 33%-C, 8-ZCBNNR with 25%-C, B-rich 6-ACBNNR with 33%-C and B-rich 8-ZCBNNR with 25%-C after $H_2S$ molecule adsorption.

| system | $E_F(eV)$ | $E_g(eV)$ | Δ(Å) | electrical conductivity |
|---|---|---|---|---|
| 6-ACBNNR with 33%-C + $H_2S$ | -3.280 | 0.857 | 0.812 | semiconductor |
| 8-ZCBNNR with 25%-C + $H_2S$ | -3.100 | 0.875 | 0.745 | semiconductor |
| B-rich 6-ACBNNR with 33%-C + $H_2S$ | -3.565 | 0 | 1.644 | metal |
| B-rich 8-ZCBNNR with 25%-C + $H_2S$ | -3.322 | 0 | 0.784 | metal |

**Table S9:** HF molecule adsorbed on 6-ACBNNR with 33%-C, 8-ZCBNNR with 25%-C, B-rich 6-ACBNNR with 33%-C and B-rich 8-ZCBNNR with 25%-C: the bond length of gas molecule (L), adsorption distance of nearest-neighbor atoms between the gas molecule and substrate (D), the angle of gas molecule ($\alpha$), charge transfer between gas molecule and substrate ($\Delta Q$), the sign "-" means that the molecule is the acceptor of the charge and the sign "+" means the molecule is the donor of the charge, and adsorption energy ($E_{ads}$). The words "before" and "after" express the characteristics of the gas molecule before and after gas molecule adsorption, respectively.

| HF molecule adsorption | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| substrate | L (Å) | | D (Å) | | $\alpha$ (°) | | $\Delta Q$ ($e$) | $E_{ads}$ ($eV$) | Type of adsorption |
| | before | after | before | after | before | after | | | |
| 6-ACBNNR with 33%-C | 0.929 | 0.939 | 3.257 | 2.143 | - | - | -0.072 | -1.541 | physisorption |
| 8-ZCBNNR with 25%-C | | 0.930 | 2.772 | 2.659 | | - | +0.031 | -0.936 | physisorption |
| B-rich 6-ACBNNR with 33%-C | | 0.933 | 2.000 | 2.640 | | - | -0.044 | -1.938 | physisorption |
| B-rich 8-ZCBNNR with 25%-C | | 0.932 | 2.000 | 2.531 | | - | +0.052 | -1.060 | physisorption |

**Table S10:** Fermi energy ($E_F$), energy band gap ($E_g$), structural deformation (Δ) and electrical conductivity of 6-ACBNNR with 33%-C, 8-ZCBNNR with 25%-C, B-rich 6-ACBNNR with 33%-C and B-rich 8-ZCBNNR with 25%-C after HF molecule adsorption.

| **system** | $\boldsymbol{E_F(eV)}$ | $\boldsymbol{E_g(eV)}$ | Δ(Å) | **electrical conductivity** |
|---|---|---|---|---|
| 6-ACBNNR with 33%-C + HF | -3.295 | 0.849 | 1.533 | semiconductor |
| 8-ZCBNNR with 25%-C + HF | -3.350 | 0.875 | 0.734 | semiconductor |
| B-rich 6-ACBNNR with 33%-C + HF | -3.569 | 0 | 1.661 | metal |
| B-rich 8-ZCBNNR with 25%-C + HF | -3.300 | 0 | 0.773 | metal |

**Table S11:** $NH_3$ molecule adsorbed on 6-ACBNNR with 33%-C, 8-ZCBNNR with 25%-C, B-rich 6-ACBNNR with 33%-C and B-rich 8-ZCBNNR with 25%-C: the bond length of gas molecule (L), adsorption distance of nearest-neighbor atoms between the gas molecule and substrate (D), the angle of gas molecule ($\alpha$), charge transfer between gas molecule and substrate ($\Delta Q$), the sign "-" means that the molecule is the acceptor of the charge and the sign "+" means the molecule is the donor of the charge, and adsorption energy ($E_{ads}$). The words "before" and "after" express the characteristics of the gas molecule before and after gas molecule adsorption, respectively.

**$NH_3$ molecule adsorption**

| **substrate** | **L (Å)** | | **D (Å)** | | **$\alpha$ (°)** | | **$\Delta Q$ ($e$)** | **$E_{ads}$ ($eV$)** | **Type of adsorption** |
|---|---|---|---|---|---|---|---|---|---|
| | **before** | **after** | **before** | **after** | **before** | **after** | | | |
| 6-ACBNNR with 33%-C | N-H1 =1.041 | N-H1 =1.042<br>N-H2 =1.041<br>N-H3 =1.041 | 2.455 | 3.077 | H1-N-H2 =105.504 | H1-N-H2 =105.788<br>H1-N-H3 =105.515<br>H2-N-H3 =105.585 | +0.030 | -1.542 | physisorption |
| 8-ZCBNNR with 25%-C | N-H2 =1.041 | N-H1 =1.043<br>N-H2 =1.042<br>N-H3 =1.039 | 2.000 | 2.884 | H1-N-H3 =105.504 | H1-N-H2 =106.068<br>H1-N-H3 =106.140<br>H2-N-H3 =105.893 | +0.034 | -0.973 | physisorption |
| B-rich 6-ACBNNR with 33%-C | N-H3 =1.041 | N-H1 =1.047<br>N-H2 =1.051<br>N-H3 =1.043 | 2.134 | 1.699 | H2-N-H3 =105.512 | H1-N-H2 =108.661<br>H1-N-H3 =108.391<br>H2-N-H3 =109.365 | +0.404 | -2.411 | chemisorption |
| B-rich 8-ZCBNNR with 25%-C | | N-H1 =1.043<br>N-H2 =1.060<br>N-H3 =1.043 | 2.133 | 1.706 | | H1-N-H2 =108.434<br>H1-N-H3 =109.162<br>H2-N-H3 =108.434 | +0.405 | -1.492 | chemisorption |

**Table S12:** Fermi energy ($E_F$), energy band gap ($E_g$), structural deformation (Δ) and electrical conductivity of 6-ACBNNR with 33%-C, 8-ZCBNNR with 25%-C, B-rich 6-ACBNNR with 33%-C and B-rich 8-ZCBNNR with 25%-C after $NH_3$ molecule adsorption.

| **system** | $\boldsymbol{E_F(eV)}$ | $\boldsymbol{E_g(eV)}$ | Δ(Å) | **electrical conductivity** |
|---|---|---|---|---|
| 6-ACBNNR with 33%-C + $NH_3$ | -3.158 | 0.857 | 1.546 | semiconductor |
| 8-ZCBNNR with 25%-C + $NH_3$ | -3.000 | 0.849 | 0.766 | semiconductor |
| B-rich 6-ACBNNR with 33%-C + $NH_3$ | -2.860 | 0 | 1.610 | metal |
| B-rich 8-ZCBNNR with 25%-C + $NH_3$ | -2.760 | 0 | 0.865 | metal |

**Table S13:** SF (sensitivity factor) for tow semiconductor structures, 6-ACBNNR with 33%-C and 8-ZCBNNR with 25%-C.

| **system** | **SF (sensitivity factor)** | **system** | **SF (sensitivity factor)** |
|---|---|---|---|
| 6-ACBNNR with 33%-C + CO | 14.98% | 8-ZCBNNR with 25%-C + CO | 3.88% |
| 6-ACBNNR with 33%-C + $CO_2$ | 14.98% | 8-ZCBNNR with 25%-C + $CO_2$ | 1.88% |
| 6-ACBNNR with 33%-C + $H_2S$ | 12.61% | 8-ZCBNNR with 25%-C + $H_2S$ | 2.88% |
| 6-ACBNNR with 33%-C + HF | 11.56% | 8-ZCBNNR with 25%-C + HF | 2.88% |
| 6-ACBNNR with 33%-C + $NH_3$ | 12.61% | 8-ZCBNNR with 25%-C + $NH_3$ | 5.77% |

**Table S14:** CO molecule adsorbed at the distance of 3 Å above 8-ZCBNNR with 25%-C : the bond length of gas molecule (L), adsorption distance of nearest-neighbor atoms between the gas molecule and substrate (D), the angle of gas molecule ($\alpha$), charge transfer between gas molecule and substrate ($\Delta Q$), the sign "-" means that the molecule is the acceptor of the charge and the sign "+" means the molecule is the donor of the charge, and adsorption energy ($E_{ads}$). The words "before" and "after" express the characteristics of the gas molecule before and after gas molecule adsorption, respectively.

| **CO molecule adsorption at the distance of 3** Å | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **substrate** | **L (Å)** | | **D (Å)** | | **$\alpha$ (°)** | | **$\Delta Q$ ($e$)** | **$E_{ads}$ ($eV$)** | **Type of adsorption** |
| | **before** | **after** | **before** | **after** | **before** | **after** | | | |
| 8-ZCBNNR with 25%-C | 1.145 | 1.149 | 3.561 | 2.958 | - | - | - 0.013 | -0.950 | physisorption |

**Table S15:** Fermi energy ($E_F$), energy band gap ($E_g$), structural deformation (Δ) and electrical conductivity of 8-ZCBNNR with 25%-C after CO molecule adsorption at the distance of 3 Å.

| **system** | **$E_F(eV)$** | **$E_g(eV)$** | Δ(Å) | **electrical conductivity** |
|---|---|---|---|---|
| 8-ZCBNNR with 25%-C + CO | -3.5 | 0.857 | 0.738 | semiconductor |

**Table S16:** $NH_3$ molecule adsorbed at the distance of 3 Å above 8-ZCBNNR with 25%-C : the bond length of gas molecule (L), adsorption distance of nearest-neighbor atoms between the gas molecule and substrate (D), the angle of gas molecule ($\alpha$), charge transfer between gas molecule and substrate ($\Delta Q$), the sign "-" means that the molecule is the acceptor of the charge and the sign "+" means the molecule is the donor of the charge, and adsorption energy ($E_{ads}$). The words "before" and "after" express the characteristics of the gas molecule before and after gas molecule adsorption, respectively.

| **$NH_3$ molecule adsorption at the distance of 3 Å** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **substrate** | **L (Å)** | | **D (Å)** | | **$\alpha$ (°)** | | **$\Delta Q$ ($e$)** | **$E_{ads}$ ($eV$)** | **Type of adsorption** |
| | **before** | **after** | **before** | **after** | **before** | **after** | | | |
| 8-ZCBNNR with 25%-C | N-H2 =1.041 | N-H1 =1.042<br>N-H2 =1.041<br>N-H3 =1.041 | 3.372 | 2.832 | H1-N-H3 =105.504 | H1-N-H2 =105.867<br>H1-N-H3 =106.093<br>H2-N-H3 =106.231 | + 0.053 | -0.907 | physisorption |

**Table S17:** Fermi energy ($E_F$), energy band gap ($E_g$), structural deformation (Δ) and electrical conductivity of 8-ZCBNNR with 25%-C after $NH_3$ molecule adsorption at the distance of 3 Å.

| **system** | **$E_F(eV)$** | **$E_g(eV)$** | Δ(Å) | **electrical conductivity** |
|---|---|---|---|---|
| 8-ZCBNNR with 25%-C + $NH_3$ | -3.00 | 0.848 | 0.755 | semiconductor |

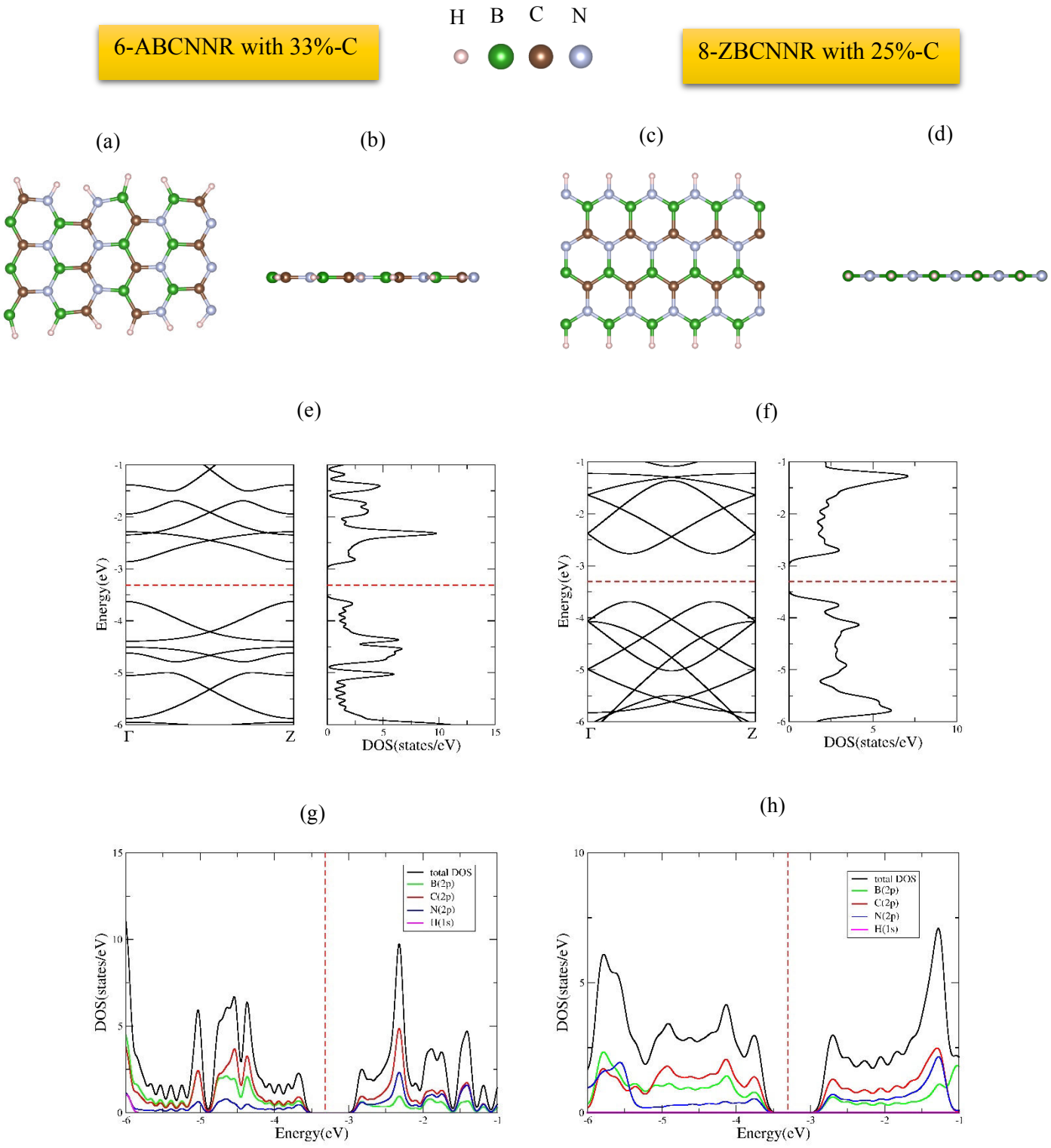


**Fig. S1** Top view and side view of the geometric configurations of 6-ACBNNR with 33%-C (a, b) and 8-ZCBNNR with 25%-C (c, d), band structure and DOS of 6-ACBNNR with 33%-C (e) and 8-ZCBNNR with 25%-C (f), PDOS of 6-ACBNNR with 33%-C (g) and 8-ZCBNNR with 25%-C (h). The Fermi level indicated by the red dashed line

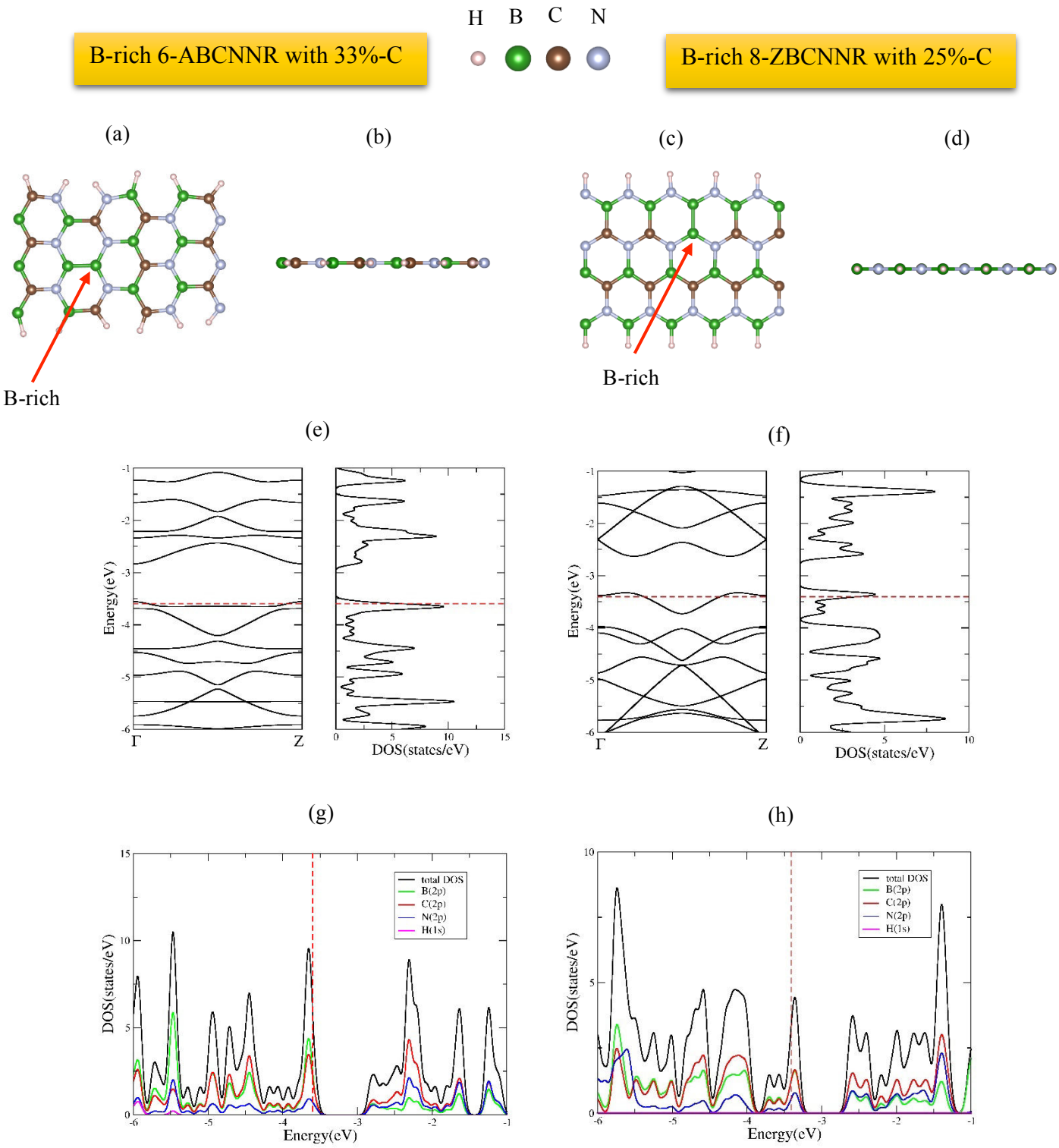


**Fig. S2** Top view and side view of the geometric configurations of B-rich 6-ACBNNR with 33%-C (a, b) and B-rich 8-ZCBNNR with 25%-C (c, d), band structure and DOS of B-rich 6-ACBNNR with 33%-C (e) and B-rich 8-ZCBNNR with 25%-C (f), PDOS of B-rich 6-ACBNNR with 33%-C (g) and B-rich 8-ZCBNNR with 50%-C (h). The Fermi level indicated by the red dashed line.

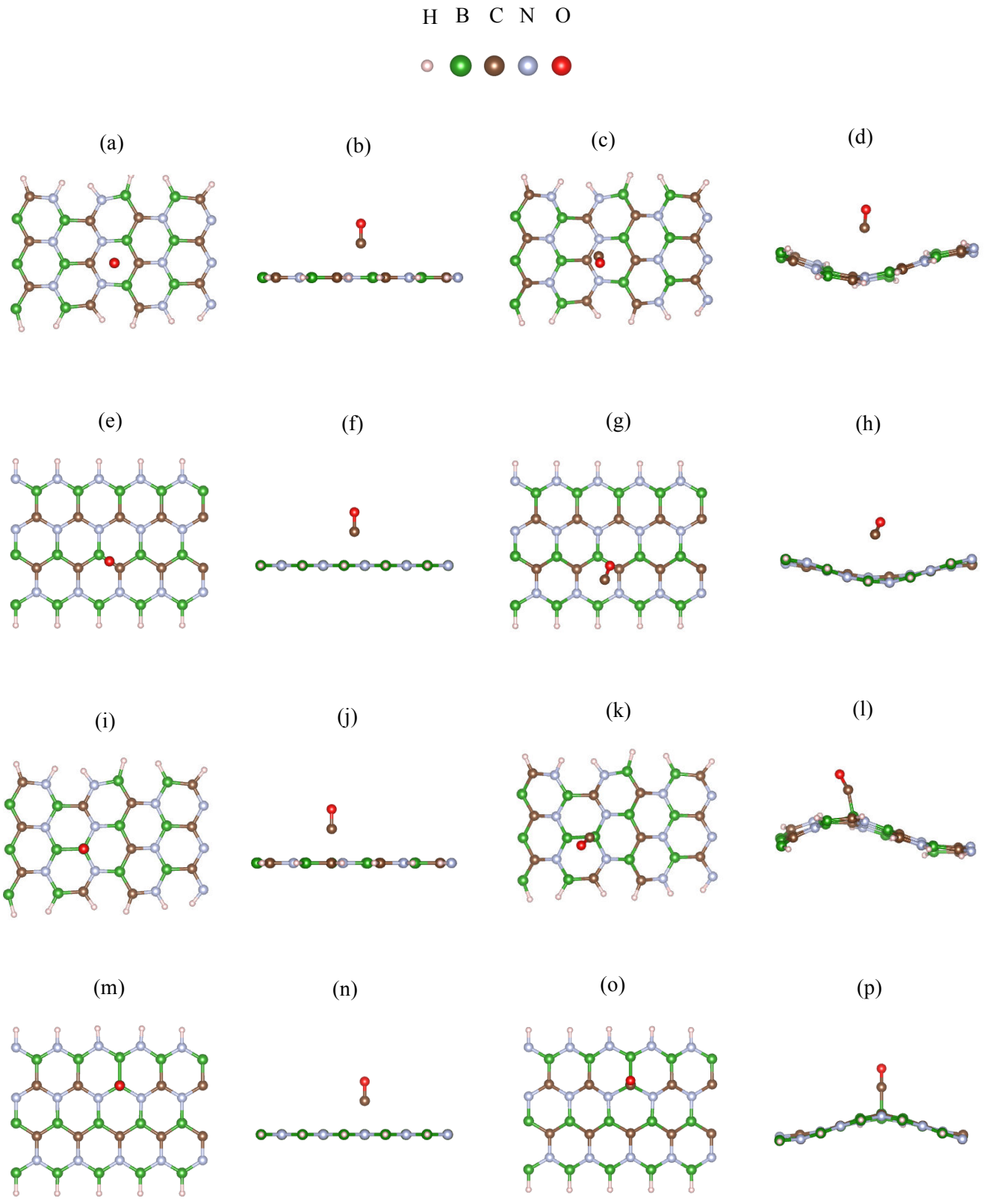


**Fig. S3** Top view and side view of the geometric configurations of CO molecule on 6-ACBNNR with 33%-C before (a, b) and after (c, d) optimization, 8-ZCBNNR with 25%-C before (e, f) and after (g, h) optimization, B-rich 6-ACBNNR with 33%-C before (i, j) and after (k, l) optimization, B-rich 8-ZCBNNR with 25%-C before (m, n) and after (o, p) optimization.

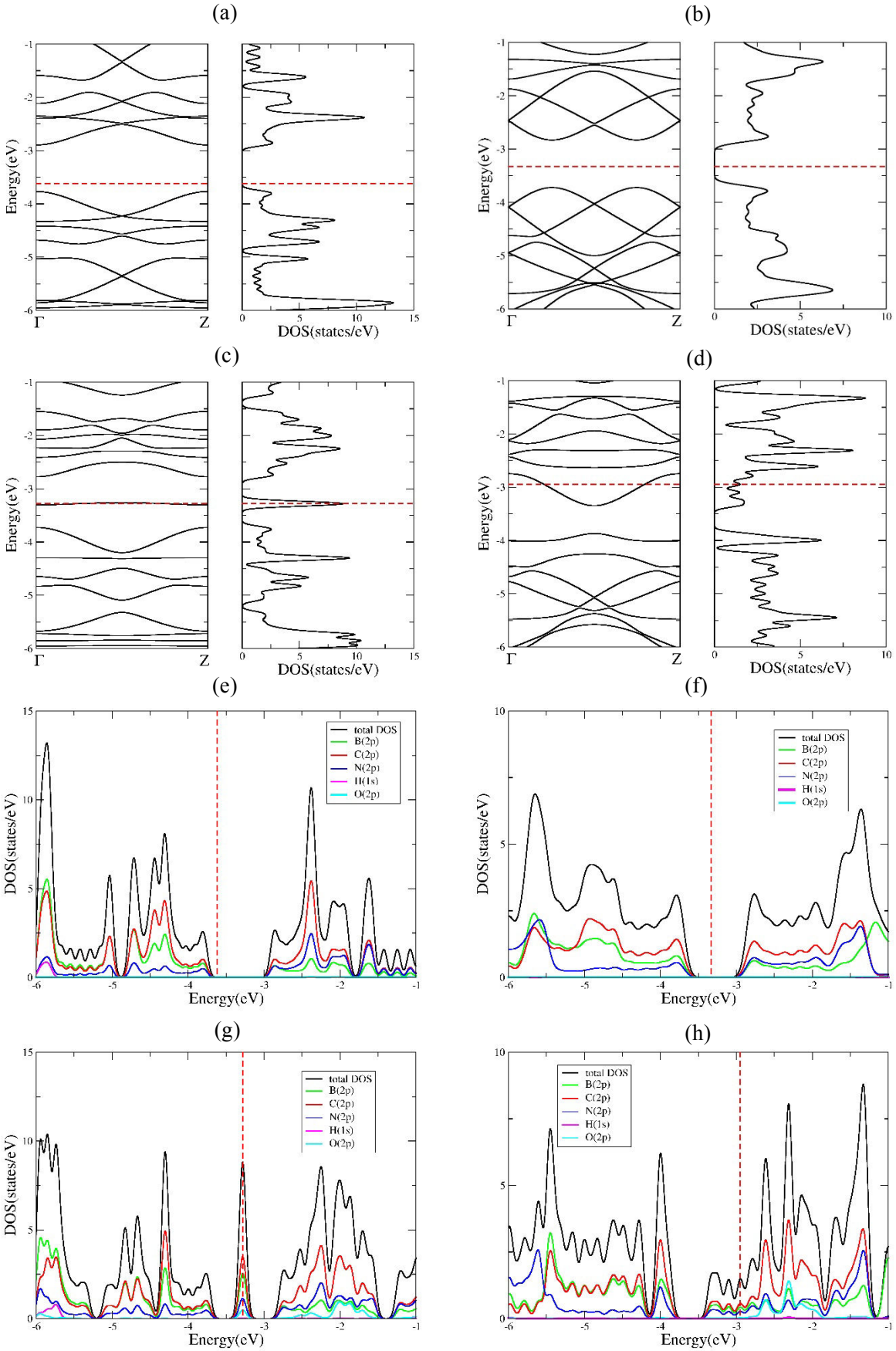


**Fig. S4** Band structure and DOS of CO molecule adsorbed on 6-ACBNNR with 33%-C (a), 8-ZCBNNR with 25%-C (b), B-rich 6-ACBNNR with 33%-C (c), B-rich 8-ZCBNNR with 25%-C (d). PDOS of CO molecule adsorbed on 6-ACBNNR with 33%-C (e), 8-ZCBNNR with 25%-C (f), B-rich 6-ACBNNR with 33%-C (g), B-rich 8-ZCBNNR with 25%-C (h). The Fermi level indicated by the red dashed line.

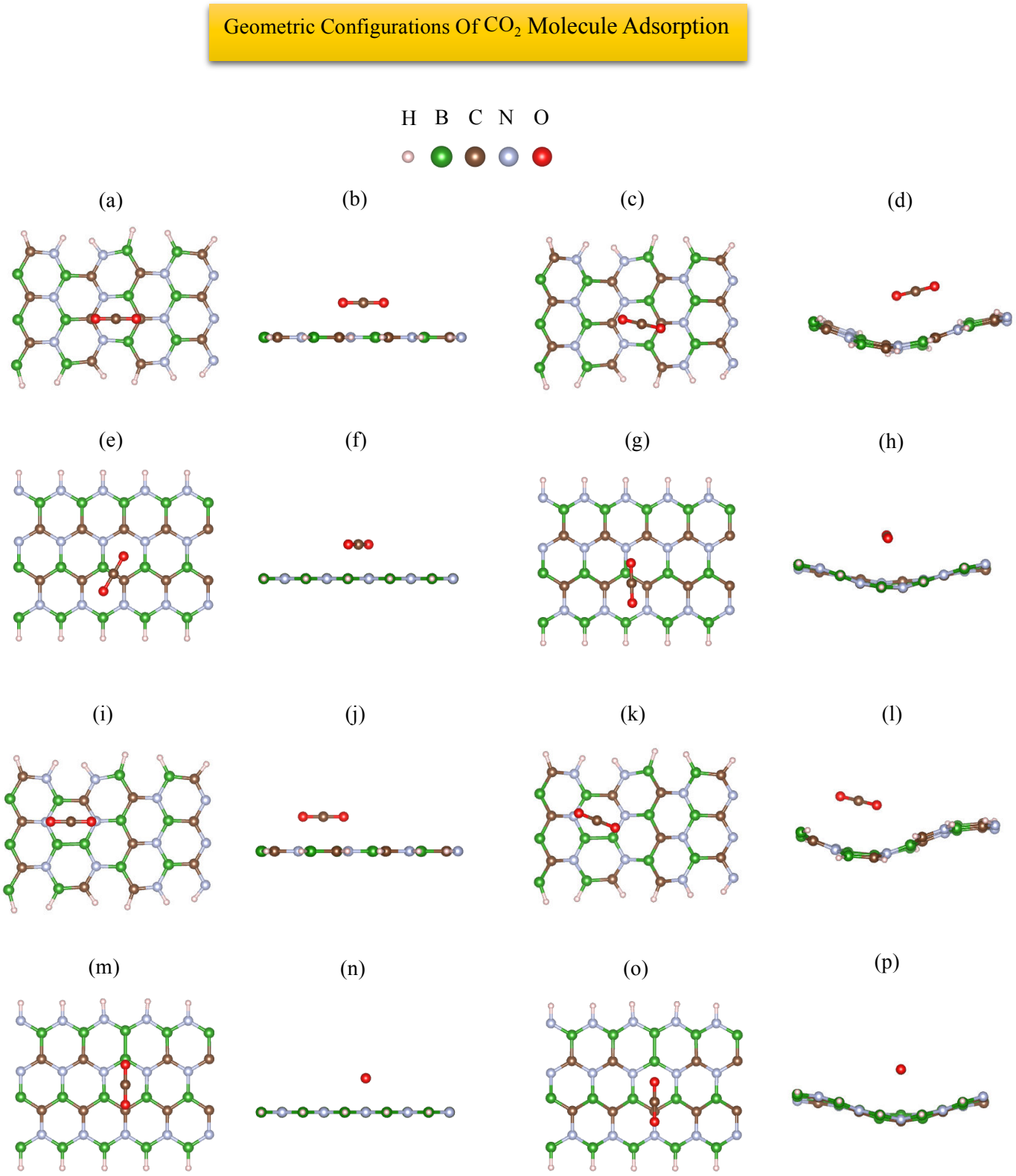


**Fig. S5** Top view and side view of the geometric configurations of $CO_2$ molecule on 6-ACBNNR with 33%-C before (a, b) and after (c, d) optimization, 8-ZCBNNR with 25%-C before (e, f) and after (g, h) optimization, B-rich 6-ACBNNR with 33%-C before (i, j) and after (k, l) optimization, B-rich 8-ZCBNNR with 25%-C before (m, n) and after (o, p) optimization.

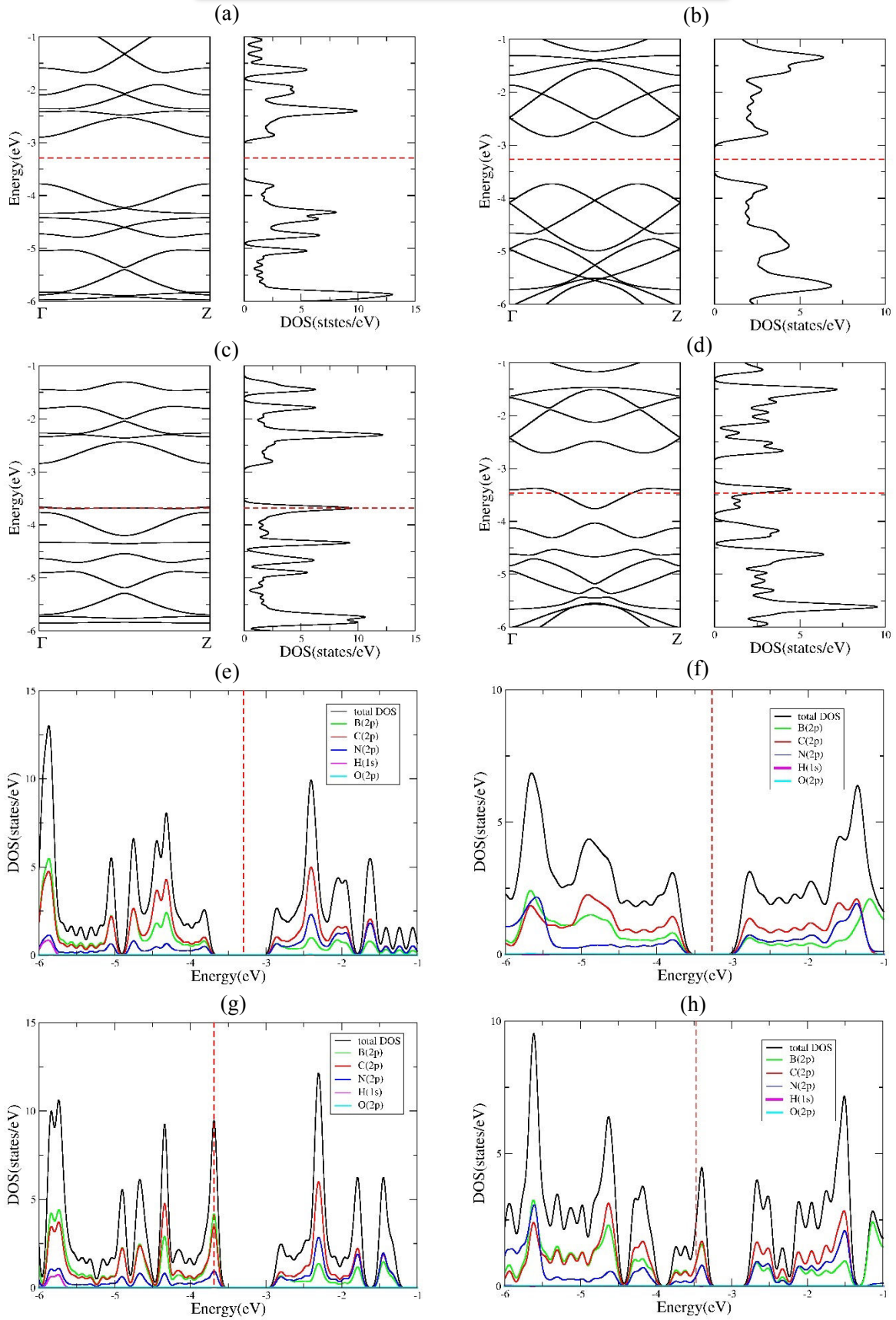


**Fig. S6** Band structure and DOS of $CO_2$ molecule adsorbed on 6-ACBNNR with 33%-C (a), 8-ZCBNNR with 25%-C (b), B-rich 6-ACBNNR with 33%-C (c), B-rich 8-ZCBNNR with 25%-C (d). PDOS of CO molecule adsorbed on 6-ACBNNR with 33%-C (e), 8-ZCBNNR with 25%-C (f), B-rich 6-ACBNNR with 33%-C (g), B-rich 8-ZCBNNR with 25%-C (h). The Fermi level indicated by the red dashed line

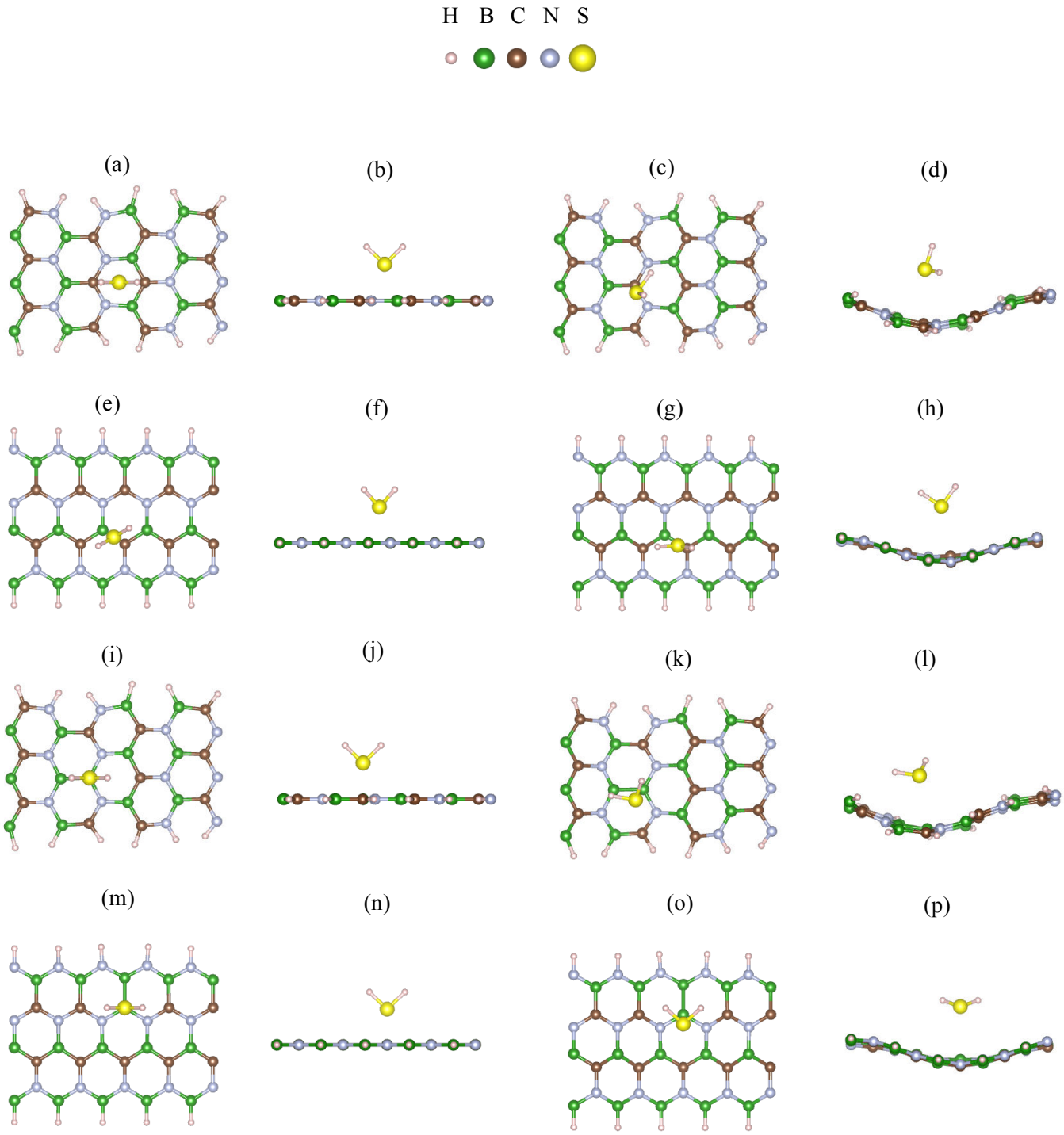


**Fig. S7** Top view and side view of the geometric configurations of $H_2S$ molecule on 6-ACBNNR with 33%-C before (a, b) and after (c, d) optimization, 8-ZCBNNR with 25%-C before (e, f) and after (g, h) optimization, B-rich 6-ACBNNR with 33%-C before (i, j) and after (k, l) optimization, B-rich 8-ZCBNNR with 25%-C before (m, n) and after (o, p) optimization.

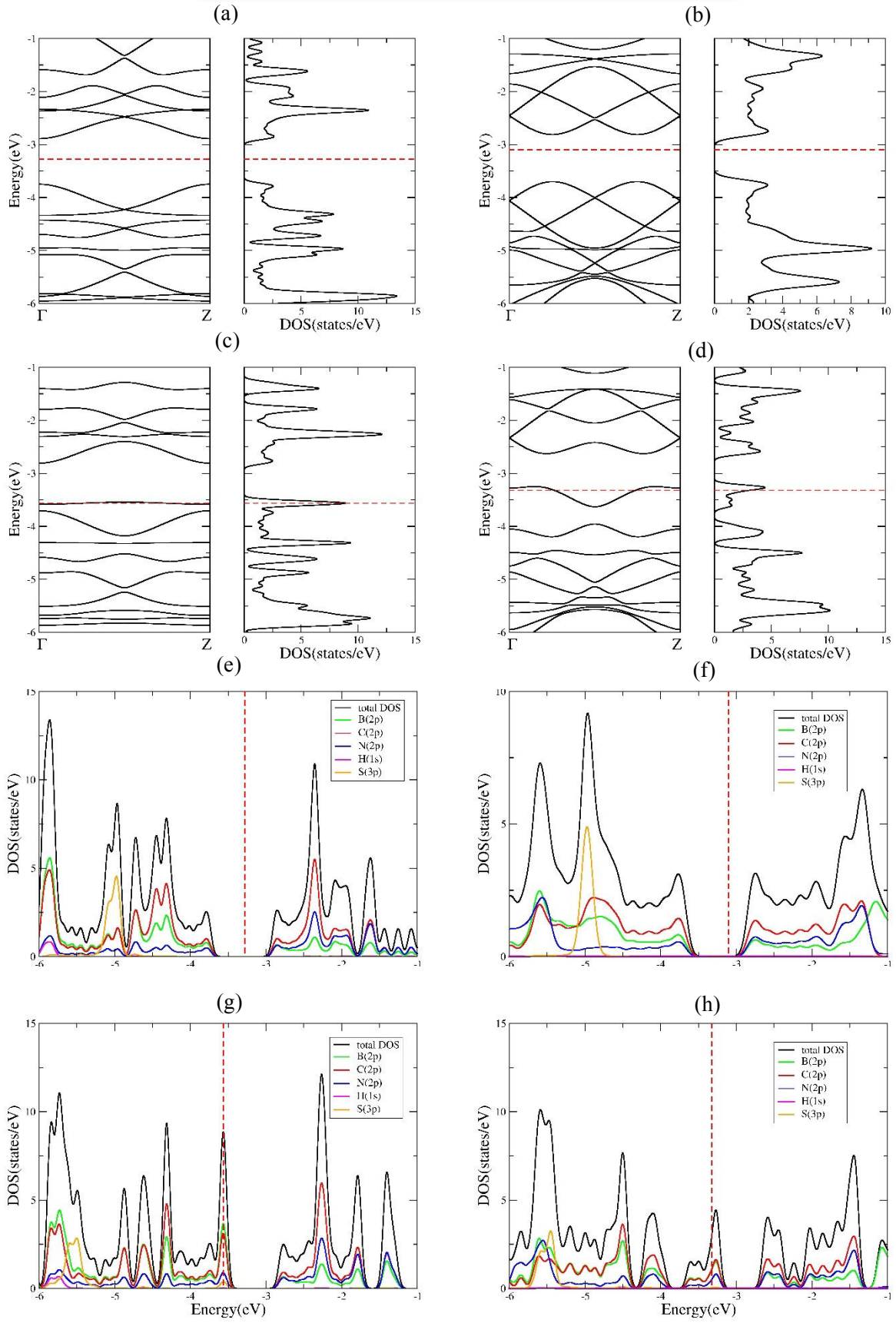


**Fig. S8** Band structure and DOS of $H_2S$ molecule adsorbed on 6-ACBNNR with 33%-C (a), 8-ZCBNNR with 25%-C (b), B-rich 6-ACBNNR with 33%-C (c), B-rich 8-ZCBNNR with 25%-C (d). PDOS of CO molecule adsorbed on 6-ACBNNR with 33%-C (e), 8-ZCBNNR with 25%-C (f), B-rich 6-ACBNNR with 33%-C (g), B-rich 8-ZCBNNR with 25%-C (h). The Fermi level indicated by the red dashed line.

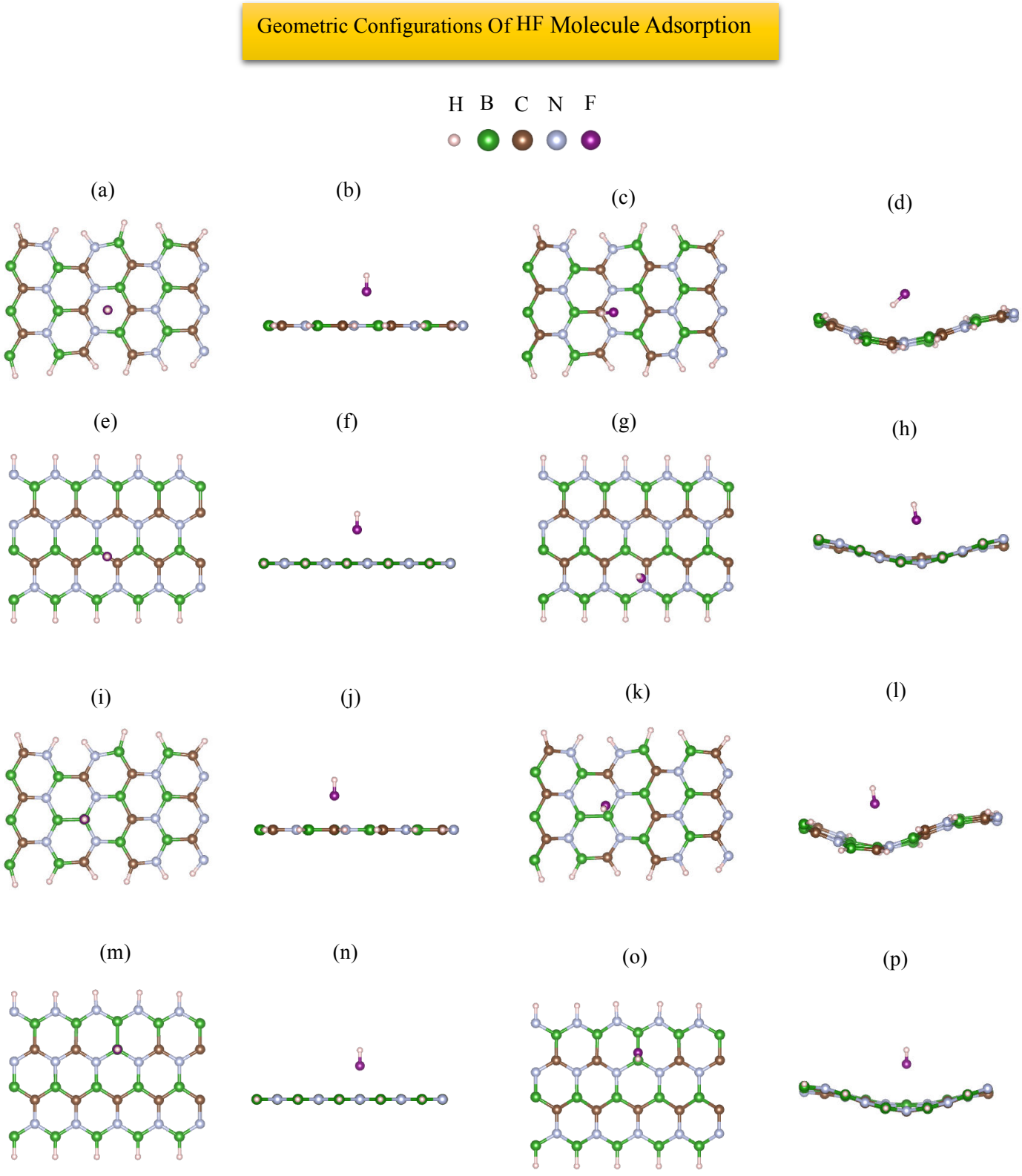


**Fig. S9** Top view and side view of the geometric configurations of HF molecule on 6-ACBNNR with 33%-C before (a, b) and after (c, d) optimization, 8-ZCBNNR with 25%-C before (e, f) and after (g, h) optimization, B-rich 6-ACBNNR with 33%-C before (i, j) and after (k, l) optimization, B-rich 8-ZCBNNR with 25%-C before (m, n) and after (o, p) optimization.

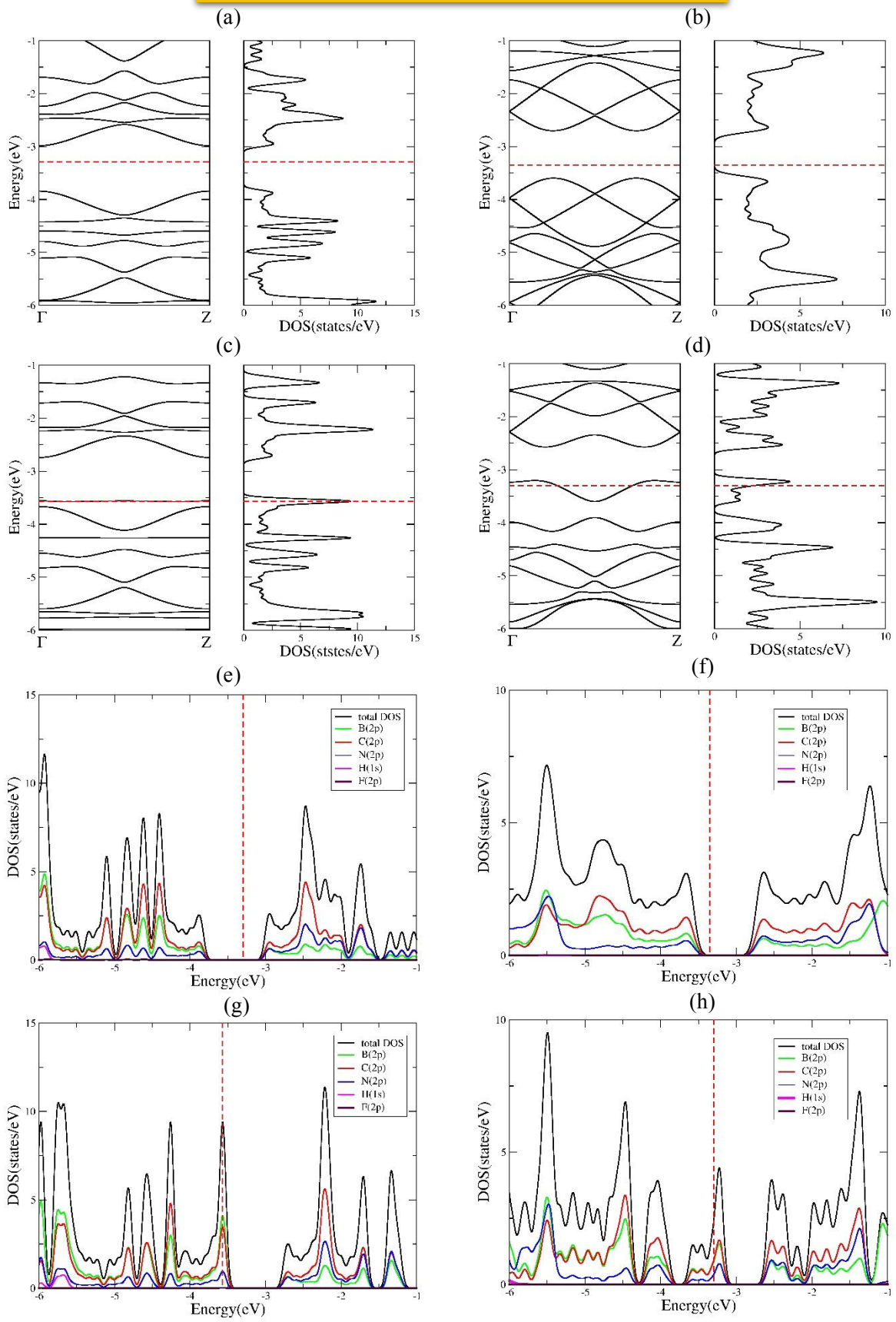


**Fig. S10** Band structure and DOS of HF molecule adsorbed on 6-ACBNNR with 33%-C (a), 8-ZCBNNR with 25%-C (b), B-rich 6-ACBNNR with 33%-C (c), B-rich 8-ZCBNNR with 25%-C (d). PDOS of CO molecule adsorbed on 6-ACBNNR with 33%-C (e), 8-ZCBNNR with 25%-C (f), B-rich 6-ACBNNR with 33%-C (g), B-rich 8-ZCBNNR with 25%-C (h). The Fermi level indicated by the red dashed line.

Geometric Configurations Of $NH_3$ Molecule Adsorption

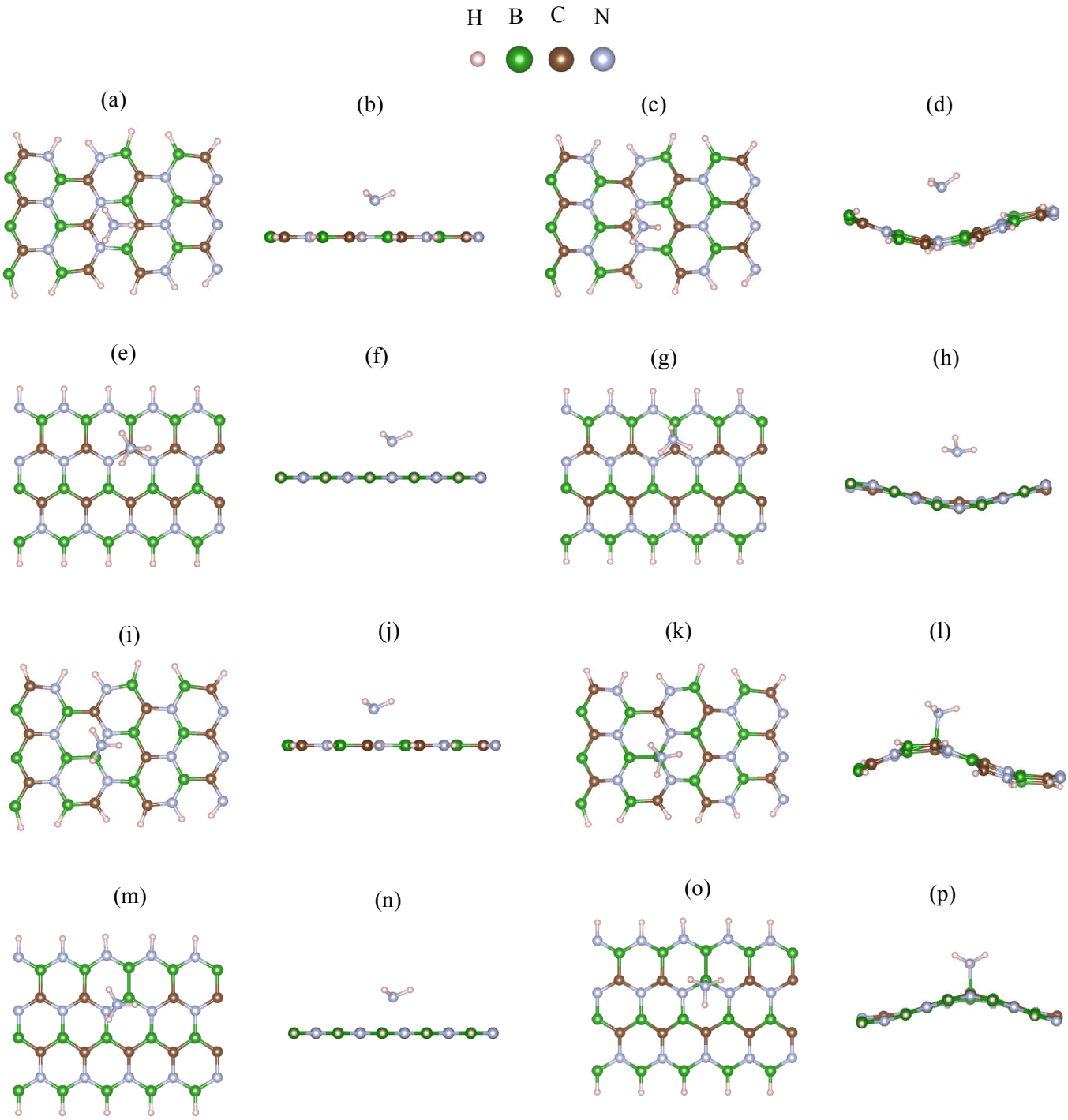


**Fig. S11** Top view and side view of the geometric configurations of $NH_3$ molecule on 6-ACBNNR with 33%-C before (a, b) and after (c, d) optimization, 8-ZCBNNR with 25%-C before (e, f) and after (g, h) optimization, B-rich 6-ACBNNR with 33%-C before (i, j) and after (k, l) optimization, B-rich 8-ZCBNNR with 25%-C before (m, n) and after (o, p) optimization.

## Electronic Properties Of $NH_3$ Molecule Adsorption

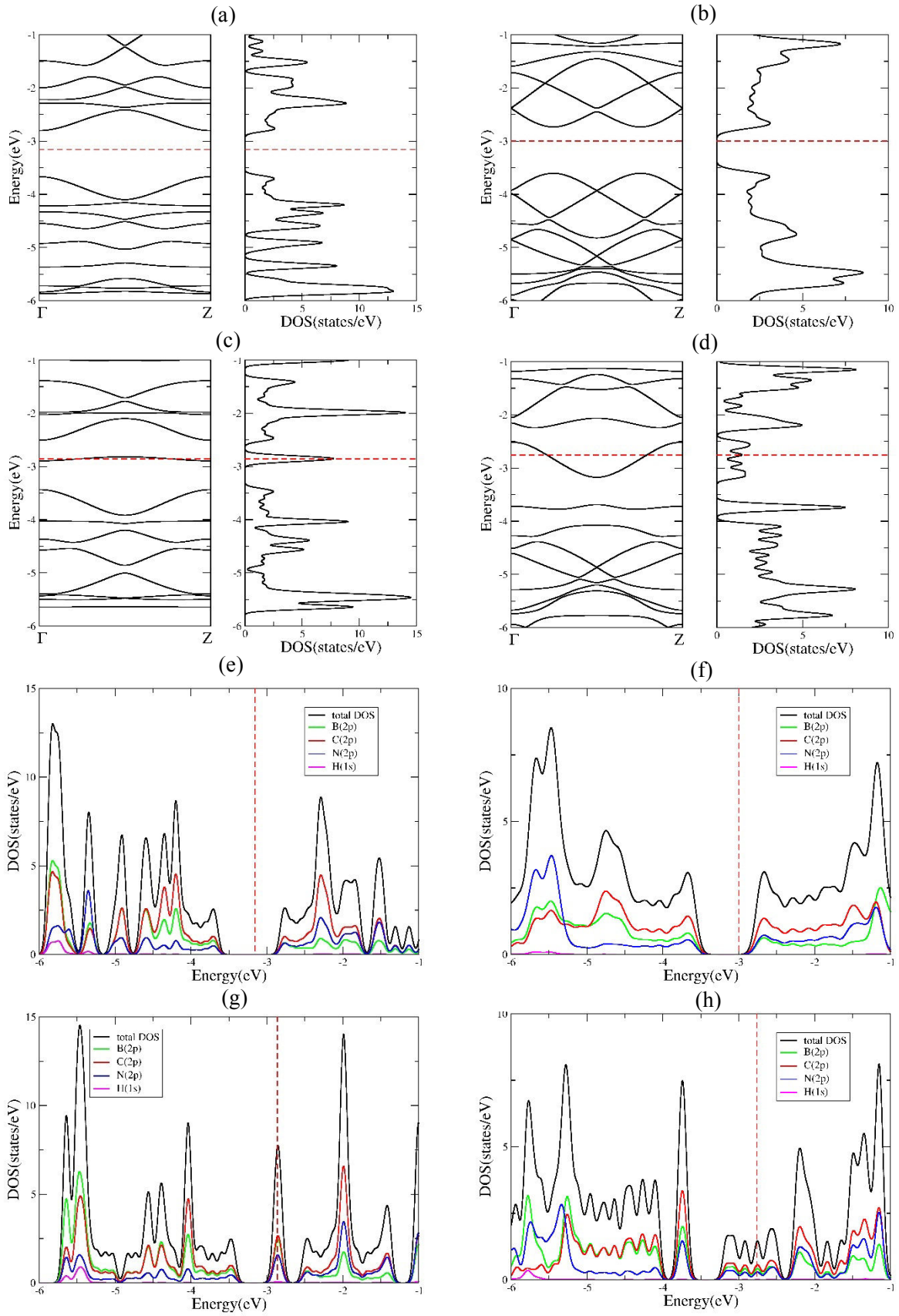


**Fig. S12** Band structure and DOS of $NH_3$ molecule adsorbed on 6-ACBNNR with 33%-C (a), 8-ZCBNNR with 25%-C (b), B-rich 6-ACBNNR with 33%-C (c), B-rich 8-ZCBNNR with 25%-C (d). PDOS of CO molecule adsorbed on 6-ACBNNR with 33%-C (e), 8-ZCBNNR with 25%-C (f), B-rich 6-ACBNNR with 33%-C (g), B-rich 8-ZCBNNR with 25%-C (h). The Fermi level indicated by the red dashed line.

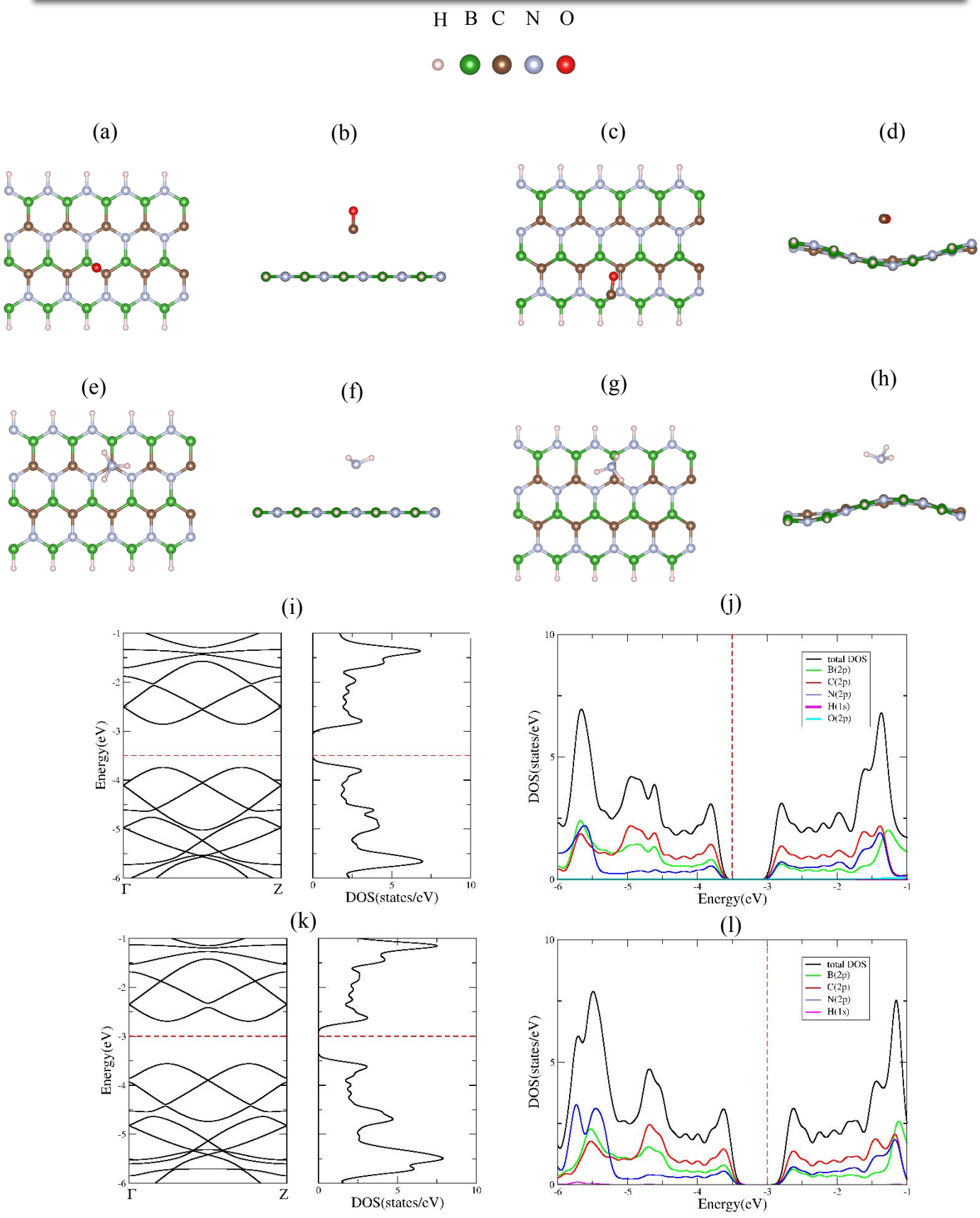


**Fig. S13** Investigation of adsorption of molecule at the distance of 3 Å above nanoribbon: Top view and side view of the geometric configurations of CO molecule on 8-ZCBNNR with 25%-C before (a, b) and after (c, d) optimization and top view and side view of the geometric configurations of $NH_3$ molecule on 8-ZCBNNR with 25%-C before (e, f) and after (g, h) optimization. (i) Band structure and DOS and (j) PDOS of CO molecule adsorbed on 8-ZCBNNR with 25%-C. (k) Band structure and DOS and (l) PDOS of $NH_3$ molecule adsorbed on 8-ZCBNNR with 25%-C. The Fermi level indicated by the red dashed line.

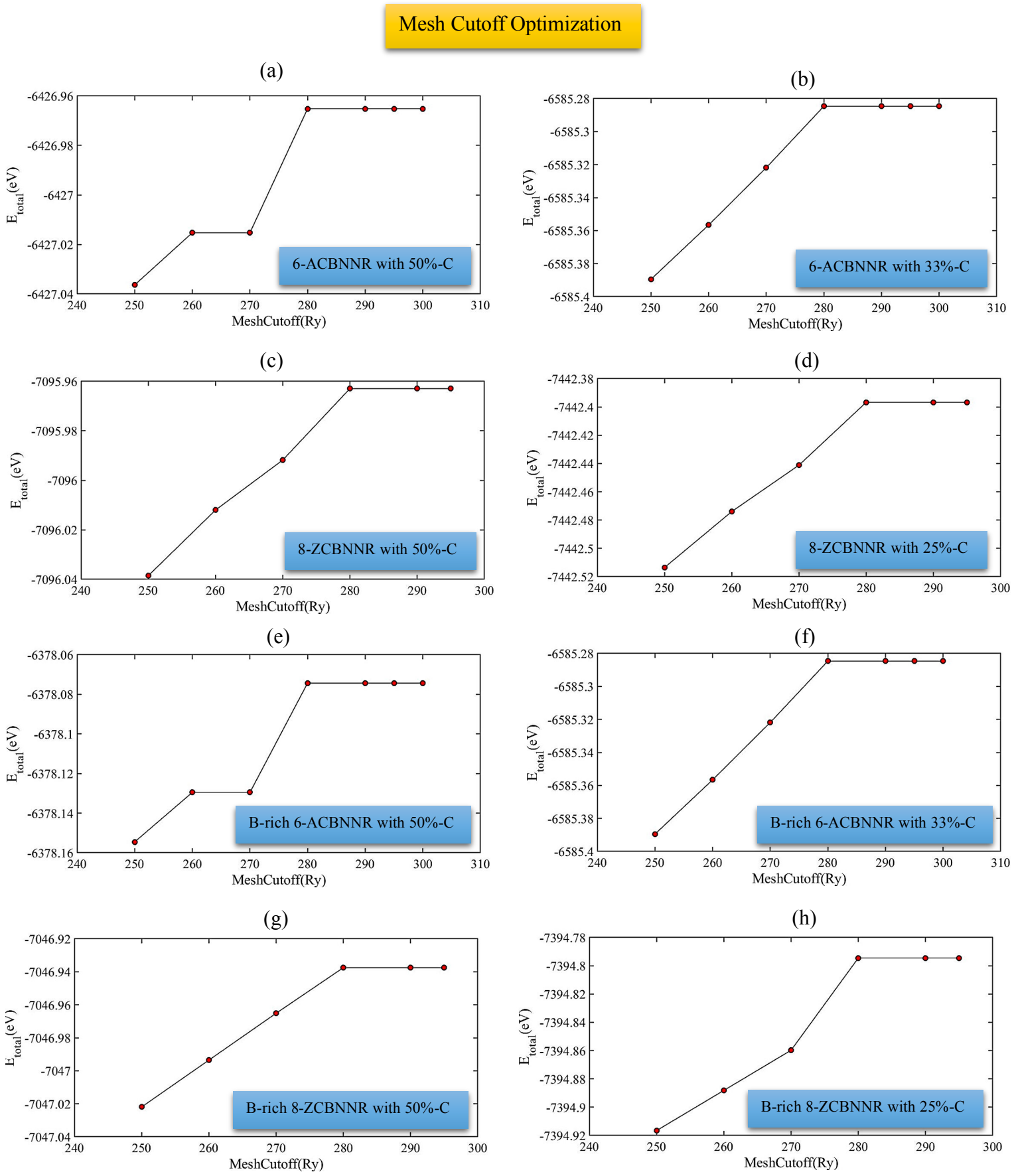


**Fig. S14** The optimized mesh cutoff energy of 6-ACBNNR with 50%-C (a), 6-ACBNNR with 33%-C (b), 8-ZCBNNR with 50%-C (c), 8-ZCBNNR with 25%-C (d), B-rich 6-ACBNNR with 50%-C (e), B-rich 6-ACBNNR with 33%-C (f), B-rich 8-ZCBNNR with 50%-C (g) and B-rich 8-ZCBNNR with 25%-C (h). For all nanoribbons, the optimized mesh cutoff energy is set at 280 Ry.