Supporting Information

CO_2 Capture on h-BN Sheet with High Selectivity Controlled by External Electric Field

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Table S1 Computed binding energies (in the unit of eV) at various adsorption configurations of CO_2 adsorbed on *h*-BN sheet.

CO_2 orientation	Hollow	topN	topB	bridgeBN
parallel	0.37	0.42	0.41	0.42
vertical	0.19	0.18	0.17	0.44

Table S2 Computed binding energies (in the unit of eV) at various adsorption configurations of H_2 adsorbed on *h*-BN sheet.

H_2 orientation	Hollow	topN	topB	bridgeBN
parallel	0.12	0.12	0.12	0.11
vertical	0.12	0.13	0.12	0.08

Table S3 Computed binding energies (in the unit of eV) at various adsorption configurations of CH_4 adsorbed on *h*-BN sheet. H_1 represents one H atom of CH_4.

CH_4 orientation	Hollow	topN	topB	bridgeBN
H_1-up	0.14	0.32	0.34	0.33
H_1-down	0.30	0.31	0.28	0.28

Table S4 Computed binding energies (in the unit of eV) at various adsorption configurations of N_2 adsorbed on *h*-BN sheet.

N_2 orientation	Hollow	topN	topB	bridgeBN
parallel	0.08	0.23	0.24	0.12
vertical	0.14	0.02	0.13	0.24

Table S5 Computed binding energies (in the unit of eV) at various adsorption configurations of CO adsorbed on *h*-BN sheet.

CO orientation	Hollow	topN	topB	bridgeBN
parallel	0.22	0.20	0.18	0.12
vertical	0.10	0.11	0.12	0.26

Table S6 Computed binding energies (in the unit of eV) at various adsorption configurations of H_2O adsorbed on *h*-BN sheet.

H_2O orientation	Hollow	topN	topB	bridgeBN
H-up	0.12	0.12	0.12	0.12
H-down	0.16	0.16	0.17	0.18