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

Supporting Information

A Computational Study of Carbon Dioxide Adsorption on Solid Boron

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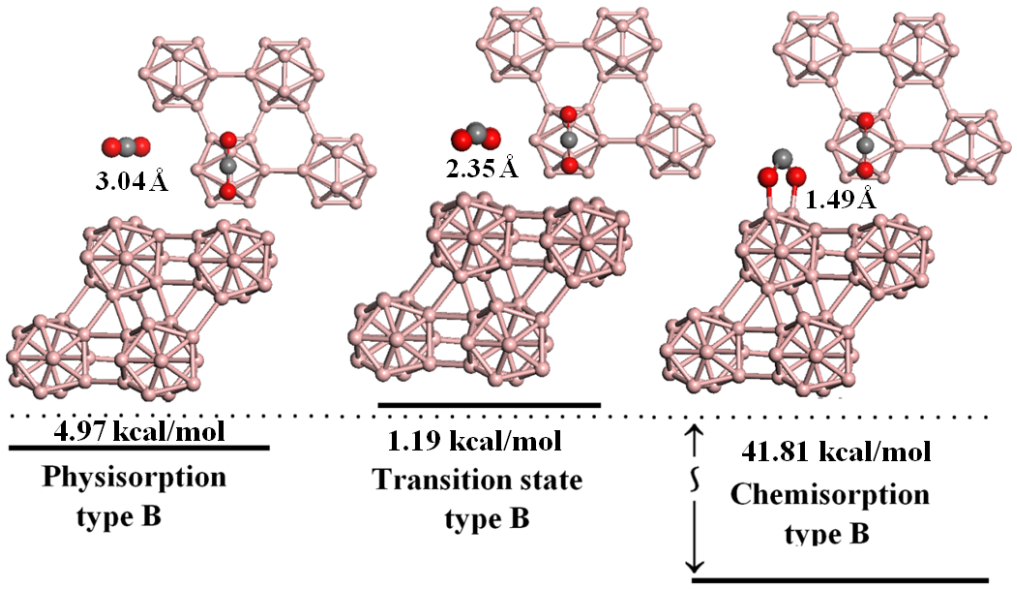
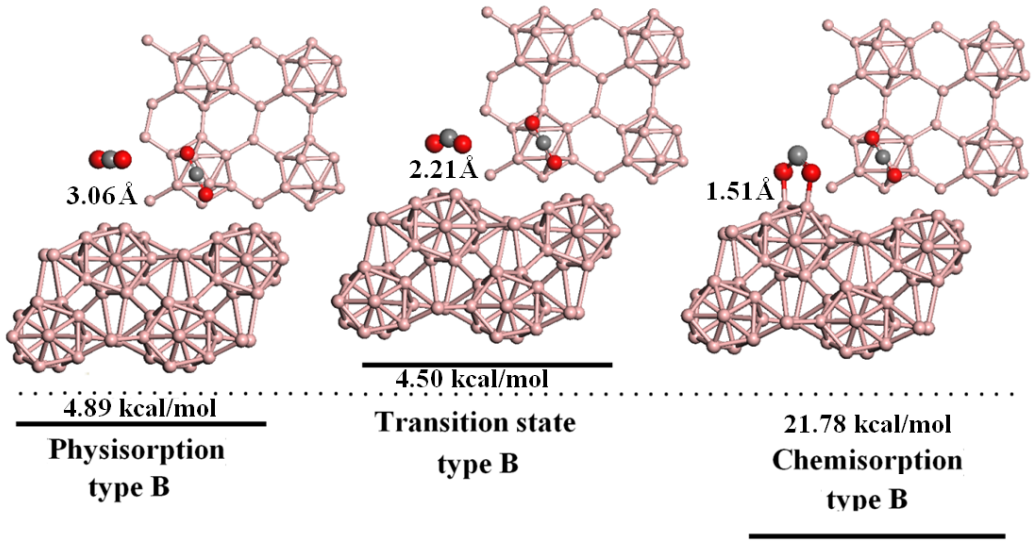


(a)



(b)

Fig. S1 Computed minimum energy configurations and transition state of CO_2 adsorption on (a) α-B_{12} and (b) γ-B_{28} surfaces involving type B interactions (top and side view of two adsorptions and transition state).

Table S1 Adsorption energy in kcal/mol, bond distance (r) in Å, bond angle (α) in deg and charge transfer (CT) in electron for the type B of CO_2 adsorption on α-B_{12} and γ-B_{28} surfaces.

		Phys	TS	Chem
α-B_{12}	Adsorption energy	-4.97	1.19	-41.81
	r(B–O)	3.013	2.350	1.494
	r(C–O)	1.177	1.192	1.330
	r(B–B)	1.598	1.624	1.683
	α(O–C–O)	179.8	157.7	115.4
	CT	0.003	-0.029	-0.606
γ-B_{28}	Adsorption energy	-4.89	4.50	-21.78
	r(B–O)	3.063	2.205	1.511
	r(C–O)	1.177	1.190	1.314
	r(B–B)	1.621	1.648	1.719
	α(O–C–O)	179.6	155.9	117.6
	CT	0.005	-0.01	-0.532

Table S2 The calculated topological parameters at the BCPs of CO_2 adsorption on α-B_{12} and γ-B_{28} of the type A.

Complexes	BCP[a]	ρ_{bcp}	$\nabla^2\rho_{bcp}$	V_{bcp}	G_{bcp}	H_{bcp}
(a) CO_2_α-B_{12}_Phy	O1–B	0.0088	0.0247	-0.0047	0.0055	0.0008
	C–O1	0.4359	0.4099	-1.6000	0.8513	-0.7487
(b) CO_2_α-B_{12}_TS	O1–B	0.0491	0.0577	-0.0470	0.0307	-0.0163
	C–O1	0.4126	-0.0063	-1.4206	0.7095	-0.7111
(c) CO_2_α-B_{12}_chem	C–B	0.1607	-0.1500	-0.2809	0.1217	-0.1592
	O1–B	0.1666	0.5157	-0.3739	0.2514	-0.1225
(d) CO_2_α-B_{12}_Phy	C–O1	0.2559	-0.5852	-0.4946	0.1741	-0.3205
	O1–B	0.0093	0.0238	-0.0051	0.0055	0.0004
	C–O1	0.4360	0.4145	-1.6019	0.8527	-0.7492
(e) CO_2_α-B_{12}_TS	O1–B	0.0737	0.1749	-0.1349	0.0893	-0.0456
	C–O1	0.4072	-0.1211	-1.3748	0.6722	-0.7026
(f) CO_2_α-B_{12}_chem	C–B	0.1609	-0.1788	-0.2755	0.1154	-0.1601
	O1–B	0.1632	0.5099	-0.3675	0.2474	-0.1201
	C–O1	0.2687	-0.6202	-0.5903	0.2176	-0.3727

[a] Atomic numbering refers to Fig. 4. The ρ_{bcp}, $\nabla^2\rho_{bcp}$, V_{bcp}, G_{bcp}, and H_{bcp} is electron density, the Laplacian of the electron density, potential energy density, kinetic energy density, and energy density at the BCP, respectively.