Supplementary information

Carbon phosphides: promising electric field controllable nanoporous materials for CO_2 capture and separation

Sainan Zhou[a†], Maohuai Wang[a†], Jiahui Wang[a], Huili Xin[b], Siyuan Liu[a*], Zhaojie Wang[a], Shuxian Wei[b], Xiaoqing Lu[a*]

[a] *School of Materials Science and Engineering, China University of Petroleum, Qingdao, Shandong 266580, P. R. China*

[b] *College of Science, China University of Petroleum, Qingdao, Shandong 266580, P. R. China*

* Corresponding authors: Siyuan Liu and Xiaoqing Lu

† These authors made an equal contribution to this work.

E-mail address: lsy@upc.edu.cn and luxq@upc.edu.cn

Table S1 Comparison of PC_n structural parameters between this work and previous literature.

Parameter	$PC_{0.33}$			PC_6		
	$PC_{0.33}$	Ref. 1	Error	PC_6	Ref. 2	Error
P−P (Å)	2.30	2.28	0.87%	--	--	--
P−C (Å)	1.79	1.78	0.56%	1.82	1.81	0.55%
Average C−C (Å)	--	--	--	1.43	1.41	1.39%
Thickness (Å)	1.44	1.31	9.00%	2.19	2.14	2.28%

Table S2 Comparison of cohesive energies of PC_n between our work and previous literature.

	$PC_{0.33}$	PC_1	PC_2	PC_3	PC_5	PC_6
Our work	4.12	5.27	6.14	6.45	6.93	7.05
Previous work	4.18[1]	5.28[2]	6.05[2]	6.45[2]	6.82[2]	6.97[2]
Error	1.45%	0.90%	1.47%	0.00%	1.59%	1.13%

Table S3 The optimized bond lengths (Å) of six PC_n structures.

	$PC_{0.33}$	PC_1	PC_2	PC_3	PC_5	PC_6
P−P (Å)	2.30	2.29	2.28	--	2.13	--
P−C (Å)	1.79	1.80	1.83	1.83	1.84	1.82
Average C−C (Å)	--	1.37	1.41	1.41	1.44	1.43
Thickness (Å)	1.44	2.32	1.81	0.69	1.89	2.19

Fig. S1 Snapshots of PC_5 at the equilibrium state in the electric field of (a) 0 a.u., and (b) 0.0030 a.u. with 5 ps MD simulations.

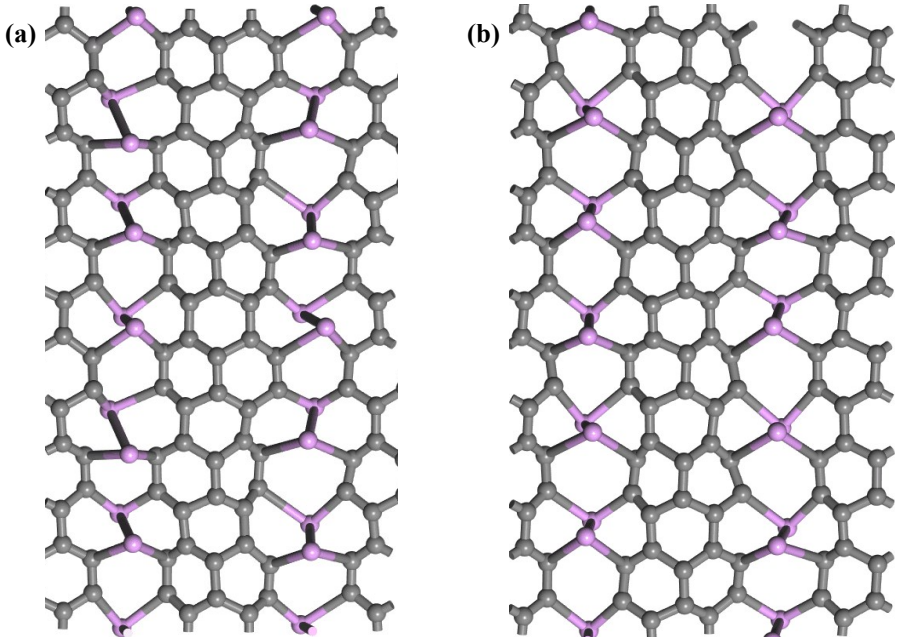


Fig. S2 The electron density distribution of their most stable adsorption configurations of CO_2/N_2/H_2O on $PC_{0.33}$ and PC_5 without an electric field. The isovalue of electron density distribution is 0.3 e/Å^3.

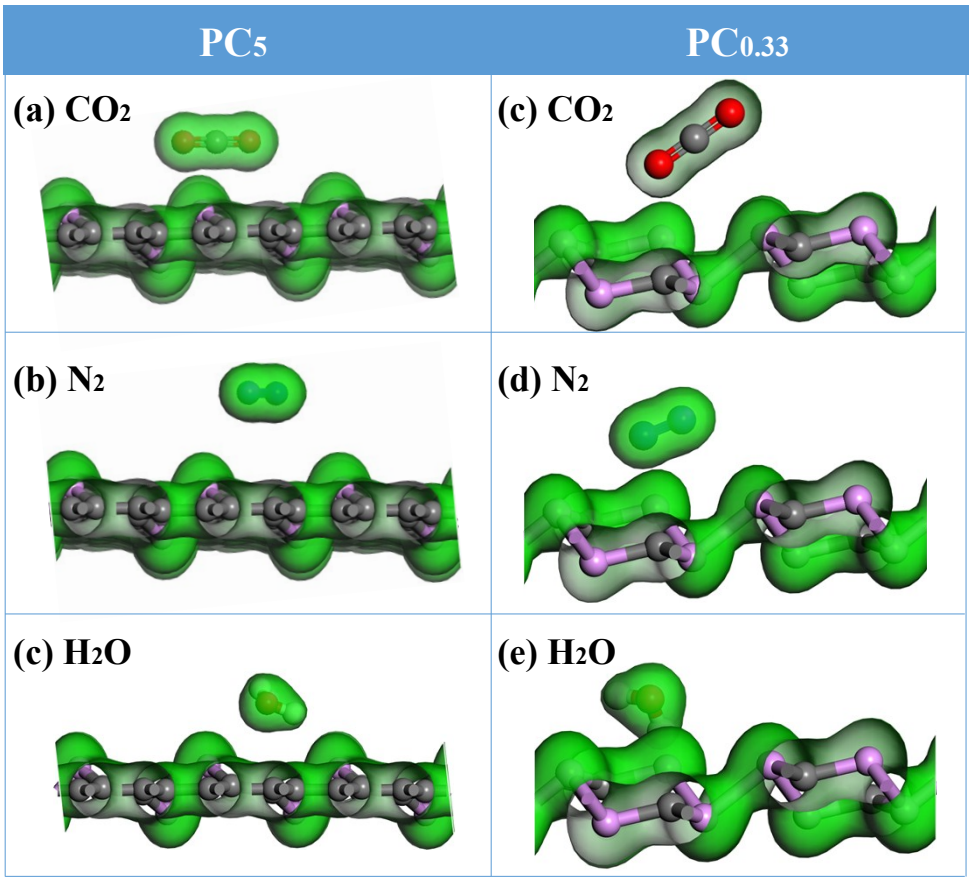


Fig. S3 The cohesive energy changes with the number of adsorption/desorption cycles.

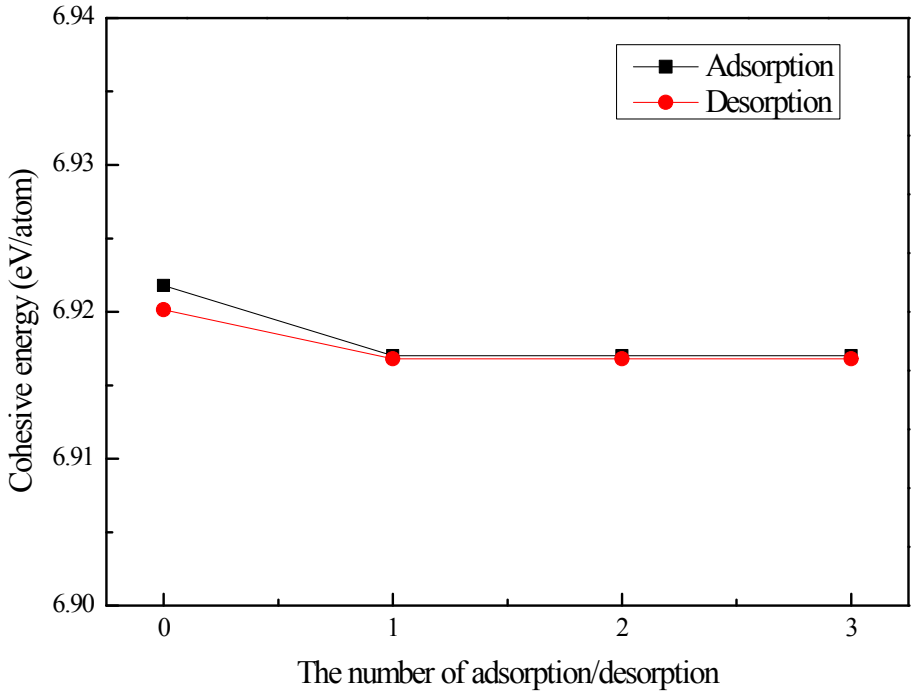


Fig. S4 Energy change of maximum CO_2adsorption capacity on PC_5 with an electric field of 0.0030 a.u.: (a) adsorption process, (b) desorption process.

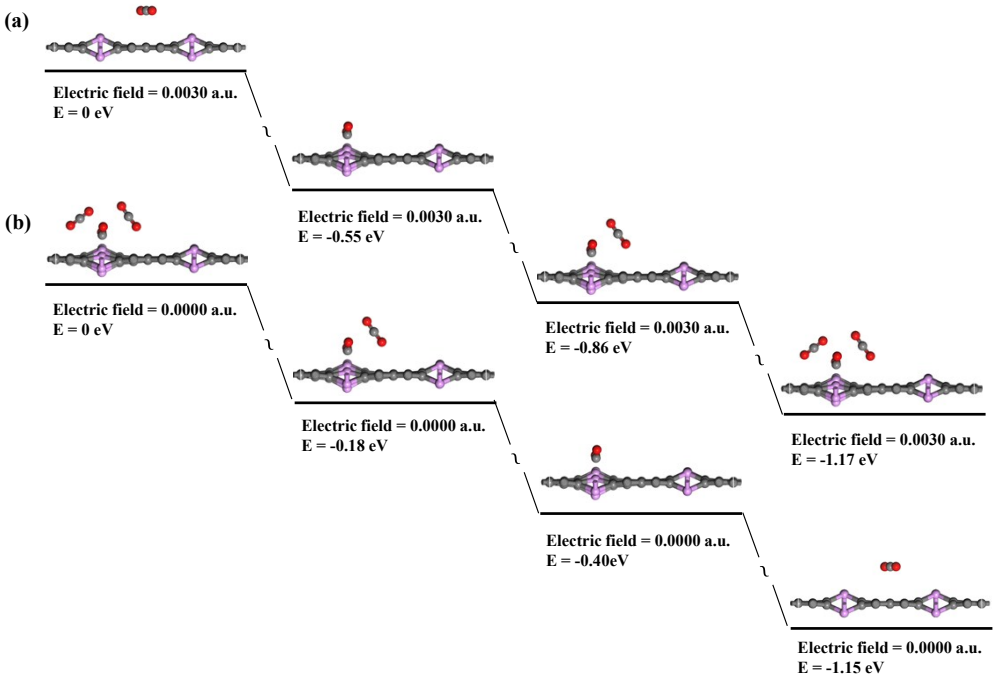
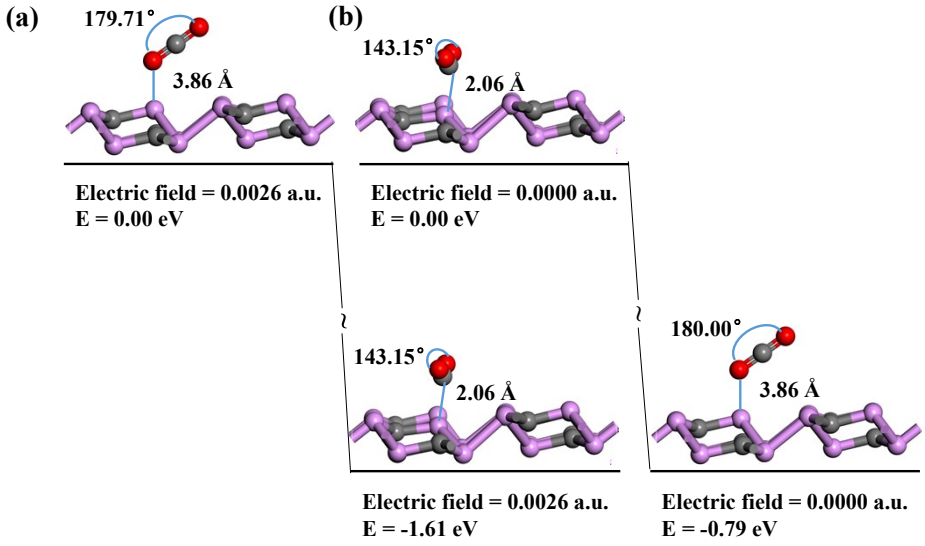


Fig. S5 Energy change of capture process of physisorbed CO_2 on PC_{033} (a) with the electric field switching on and release process of chemisorbed CO_2 from $PC_{0.33}$ (b) with the electric field switching off.



References

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2. T. Yu, Z. Zhao, Y. Sun, A. Bergara, J. Lin, S. Zhang, H. Xu, L. Zhang, G. Yang and Y. Liu, *J. Am. Chem. Soc.*, 2019, 141, 1599−1605.