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

Supporting Information

Strain Tunable CO_2 Storage by Black Phosphorene and α-PC from Combined First-principle and Molecular Dynamics Study

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1. Force Field Parameters in MD Simulations

In our simulations, the classical force field parameters for CO_2 molecules were adopted from Sandler's work which is parameterized to reproduce the experimental vapor-liquid equilibrium data.[1] Following the method of Aluru group,[2] the phosphorus and carbon atoms in BP and α-PC are described as Lennard-Jones particles. The carbon atoms in α-PC are assigned atom type "CA" in the OPLS force field with the cross section of 0.355 nm and well depth of 0.29288 kJ/mol. The phosphorus atoms in both BP and α-PC are optimized to reproduce the CO_2 adsorption energy profiles obtained from high-level quantum mechanics (QM) calculations, which are 0.377 nm (cross section) and 1.0251 kJ/mol (well-depth).

2. Energy Profiles of a CO_2 Molecule Adsorption on BP and α-PC Surface

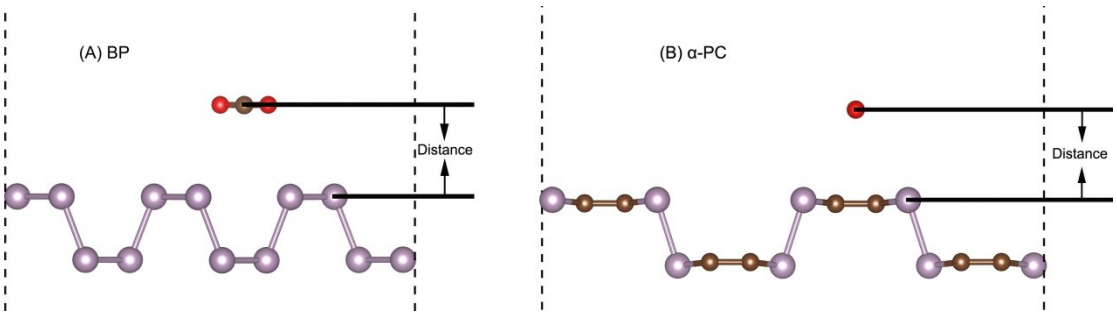

Figure s1. Illustrations of the adsorption process of a CO_2 molecule binding on (A) BP and (B) α-PC Surface.

The above parameters are optimized by reproducing the energy profiles of a CO_2 molecule adsorption on BP and α-PC Surface. Fig. s1 depicts two structure models. Using the force field parameters, the adsorption energy profiles from QM calculations are well reproduced as shown in Fig. s2.

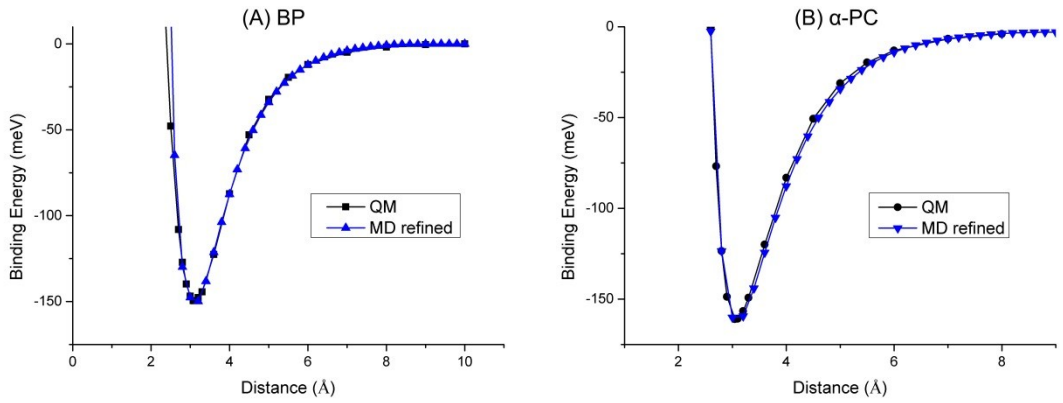

Figure s2. The energy profiles of a CO_2 molecule adsorption on (A) BP and (B) α-PC surface from quantum mechanics (QM) calculations and MD simulations with the optimized parameters.

Reference:

1. R. Babarao, Z. Hu, J. Jiang, S. Chempath and S. I. Sandler, *Langmuir*, 2007, **23**, 659-666.
2. C. Y. Won and N. R. Aluru, *Journal of the American Chemical Society*, 2007, **129**, 2748-+.