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胺基功能化的炭材料上二氧化碳吸附的密度泛函理论研究

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Density Functional Theory Study of CO_2 Adsorption in Amine-Functionalized Carbonaceous Materials

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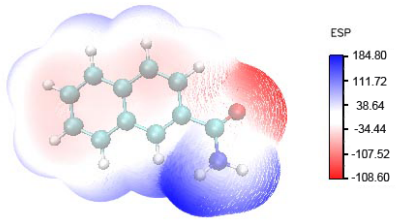

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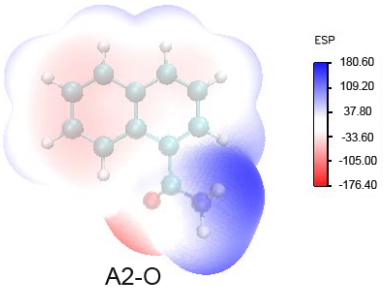

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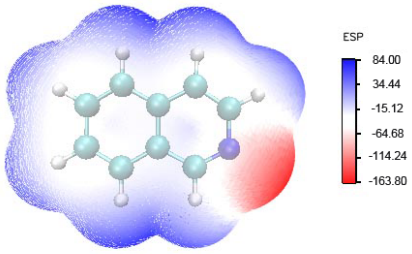

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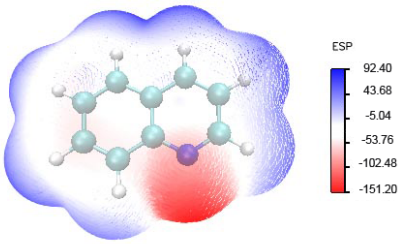

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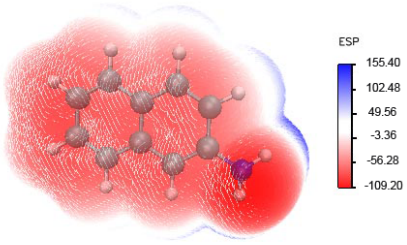

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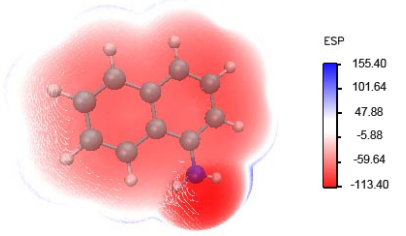

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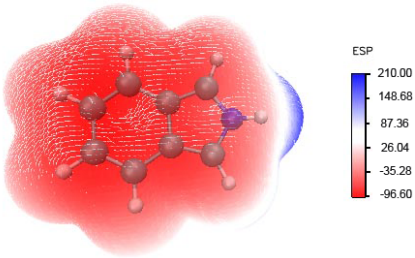

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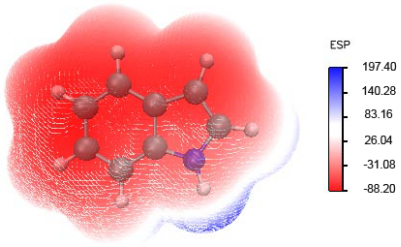

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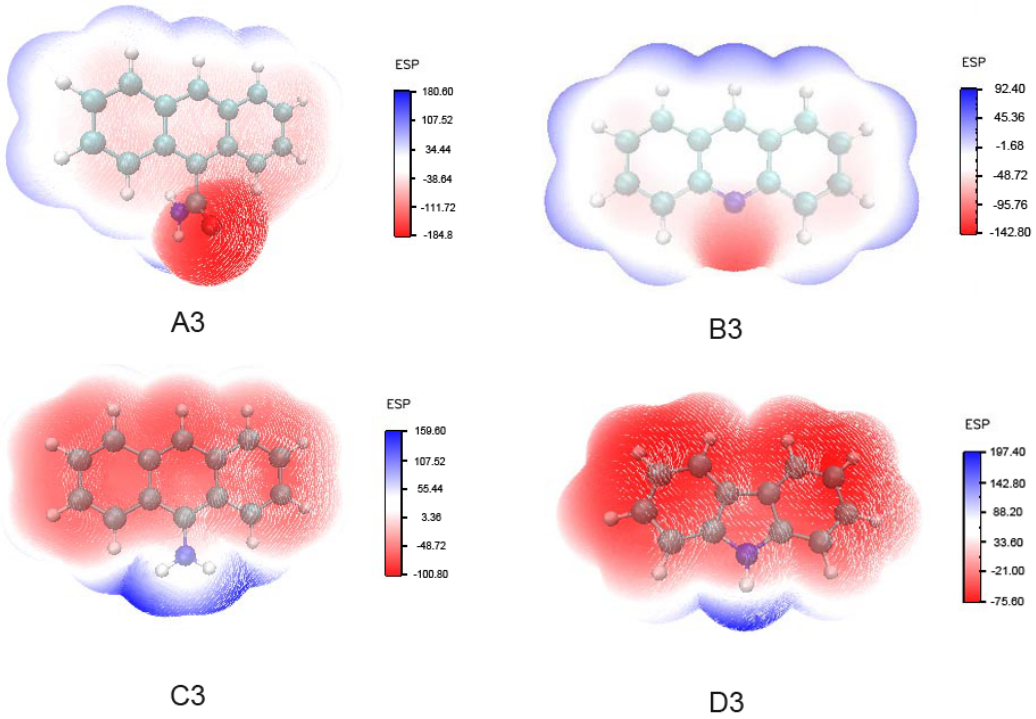
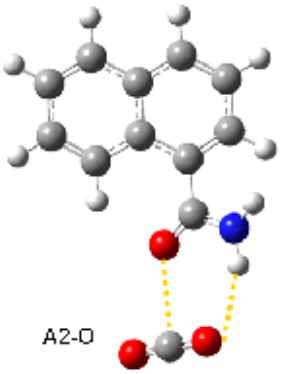


Fig.S1 Electrostatic potential isosurfaces of CO_2 and adsorbents

A1: amide-type, B1: pyridine-type, C1: aniline-type, D1: pyrrole-type adsorbent; O: ortho, M: meta, which means adding a benzene ring at the ortho or meta position on A, B, C and D. A2 and A3 mean adding one and two benzene rings on the basis of the A1 structure. The same as in B*n*, C*n* and D*n*). Red, white, and blue represent negative, zero, and positive ESP value (kJ·mol^{-1}), respectively.

A2-M



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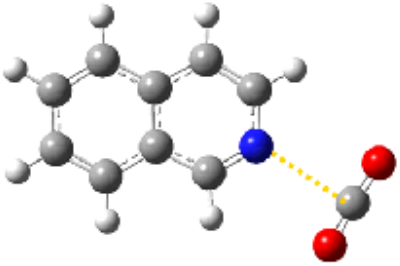

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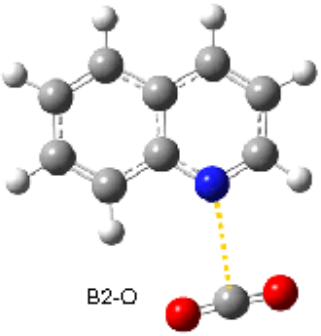

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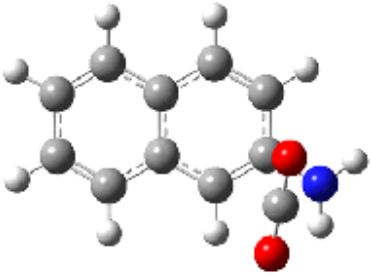

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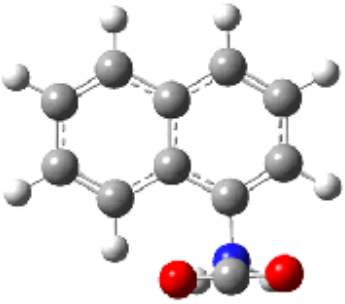

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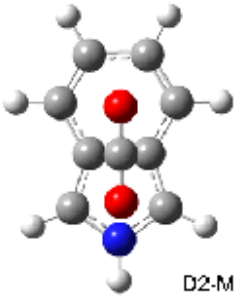

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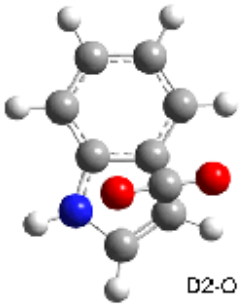

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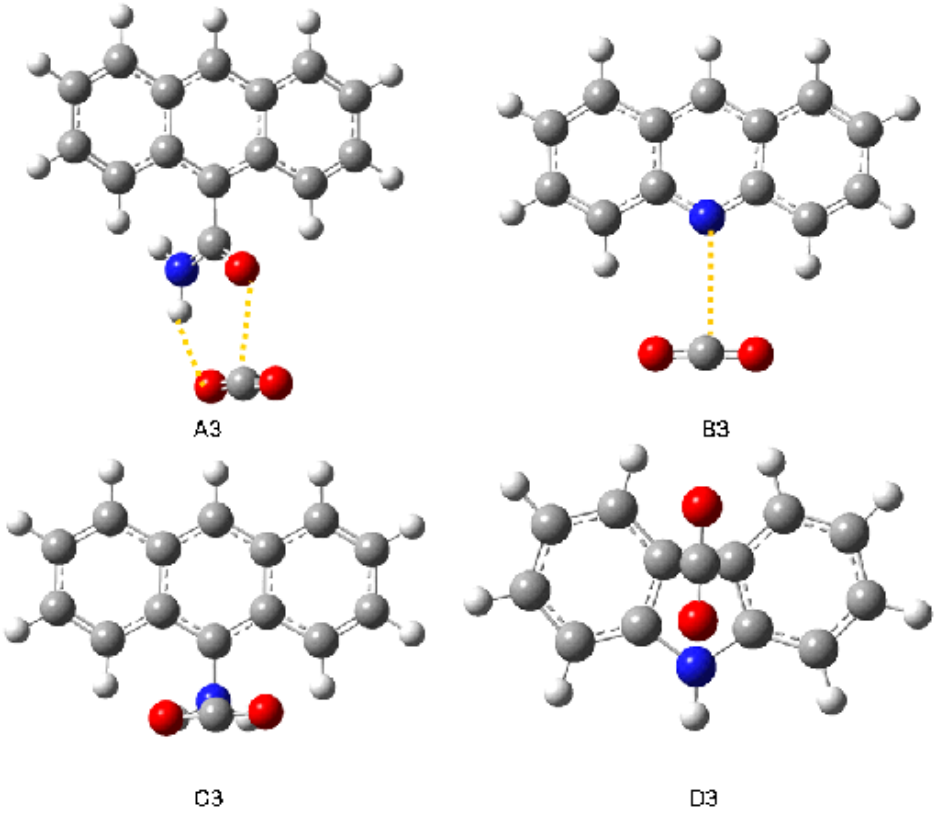
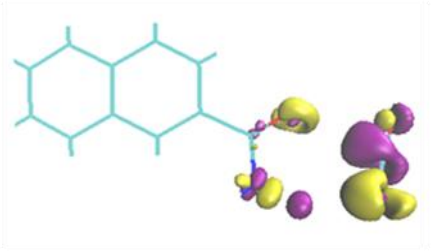


Fig.S2 Optimized geometries of CO_2-adsorbents at B3LYP-D3/6-311+G level**

A1: amide-type, B1: pyridine-type, C1: aniline-type, D1: pyrrole-type adsorbent; O: ortho, M: meta, which means adding a benzene ring at the ortho or meta position on A, B, C and D. A2 and A3 mean adding one and two benzene rings on the basis of the A1 structure. The same as in B*n*, C*n* and D*n*.



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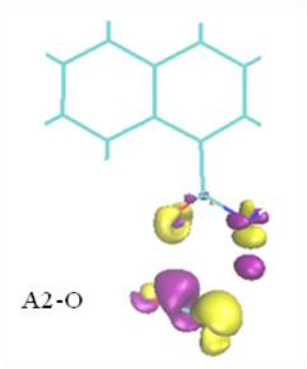

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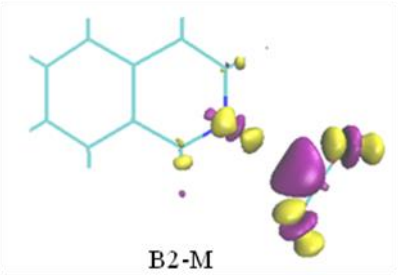

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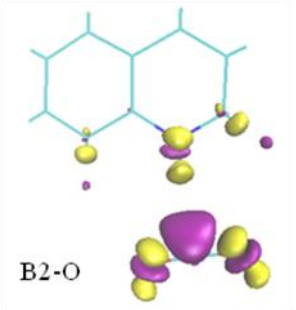

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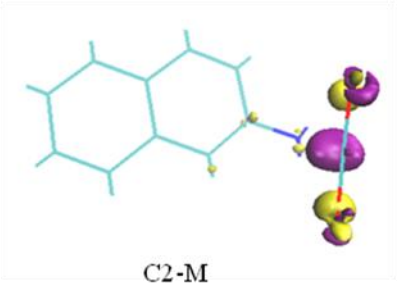
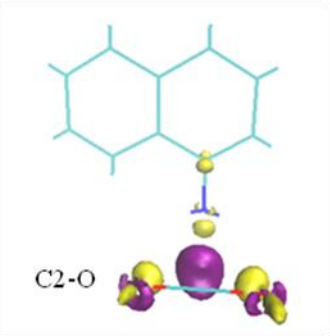


C2-M



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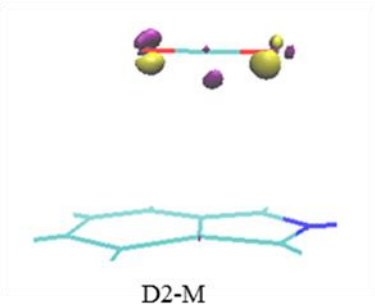

D2-M

D2-O

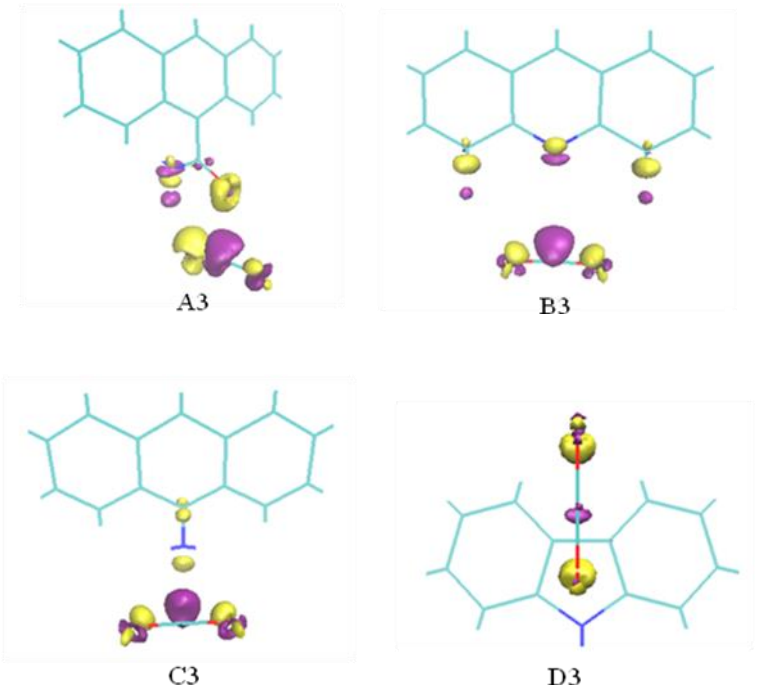

Fig.S3 Difference map of electron density of CO_2-adsorbent complexes

The purple and yellow represent the region in which electron density is decreased and increased after the adsorption, respectively. (isovalue 0.0012 a.u. A1: amide-type, B1: pyridine-type, C1: aniline-type, D1: pyrrole-type adsorbent; O: ortho, M: meta, which means adding a benzene ring at the ortho or meta position on A, B, C and D. A2 and A3 mean adding one and two benzene rings on the basis of the A1 structure. The same as in B*n*, C*n* and D*n*.

Table S1 Calculated adsorption energy (ΔE_{ad}) of CO_2 and adsorbents at B3LYP/6-311+G, B3LYP-D3/6-311+G**, M06-2X-D3/6-311+G**, ωB97XD/6-311+G** with BSSE-corrected energy at B3LYP-D3/6-311+G(*d, p*)**

	[b]ΔE_{ad}/(kJ mol^{-1}) B3LYP	ΔE_{ad}/(kJ mol^{-1}) B3LYP-D3	ΔE_{ad}/(kJ mol^{-1}) M06-2X-D3	ΔE_{ad}/(kJ mol^{-1}) ωB97XD	ΔE_{ad}/(kJ mol^{-1}) B3LYP-D3 BSSE-corrected
[a]A1	-13.6	-22.1	-23.6	-19.7	-20.8
B1	-11.3	-21.2	-23.4	-18.6	-20.0
C1	-5.0	-17.7	-20.5	-16.4	-16.0
D1	-2.9	-15.7	-18.6	-14.8	-14.4
A2-M	-13.4	-22.0	-24.7	-19.5	-20.7
A2-O	-13.1	-22.1	-24.4	-19.6	-20.8
B2-M	-11.4	-21.6	-23.6	-19.4	-20.3
B2-O	-10.8	-22.6	-24.8	-20.4	-21.1
C2-M	-3.7	-17.8	-20.5	-17.2	-16.0
C2-O	-4.1	-18.0	-20.9	-16.9	-16.3
D2-M	0.61	-16.7	-19.8	-15.5	-14.6
D2-O	-1.3	-18.0	-20.6	-16.7	-16.0
A3	-12.9	-22.1	-24.5	-19.6	-20.7
B3	-7.4	-19.4	-19.5	-17.4	-18.0
C3	-2.4	-18.2	-21.4	-17.0	-16.1
D3	-0.3	-20.0	-21.7	-18.1	-17.6

[a]A1: amide-type, B1: pyridine-type, C1: aniline-type, D1: pyrrole-type adsorbent; O: ortho, M: meta, which means adding a benzene ring at the ortho or meta position on A, B, C and D. A2 and A3 mean adding one and two benzene rings on the basis of the A1 structure. The same as in B*n*, C*n* and D*n*

[b]All energy terms are given in kJ·mol^{-1}.