Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information for

Titanium-decorated Graphene Oxide for Carbon Monoxide Capture and Separation

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Table S1 Adsorption energies (E_b) for CO, N_2, CO_2 and CH_4 on graphene are calculated by structural optimization with Drieding Force Field and compared to the experiments (graphite by expt.). Graphene is modeled by a finite molecule with 54 C atoms.

Gas	E_b (meV)	Method
CH_4	140	Expt. [a]
	142.35	Drieding
CO	109.6	Expt. [b]
	127.12	Drieding
N_2	100.9	Expt. [b]
	114.89	Drieding
CO_2	178.4	Expt. [c]
	183.43	Drieding

References:

[a] E.S. Severin and D.J. TiIdesley, Mol. Phys. 41 (1980) 1401.

[b] M.J. Bojan and W.A. Steele, Langmuir 3 (1987) 1123.

[c] R.A. Beebe, A.V. Kiselev, N.V. KovaIeva, J.R. Holmes and M.E.R. CampIin, Russ. J. Phys. Chem. 38 (1964) 506.

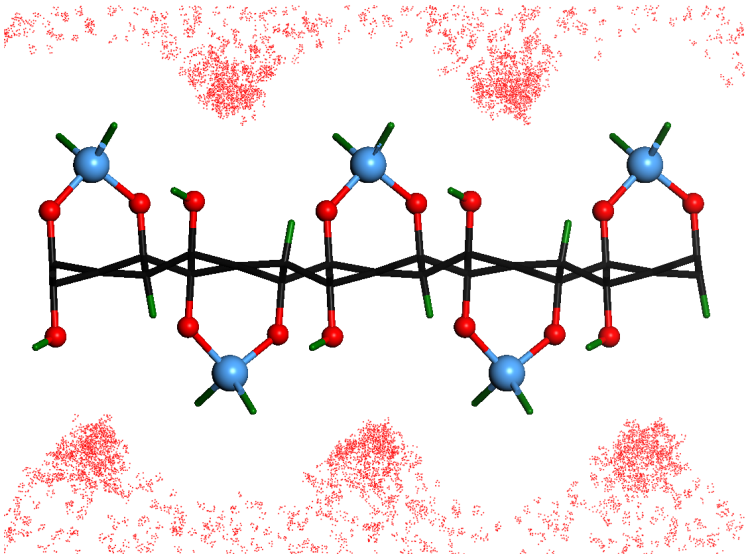

Fig. S1 Density distribution for CO_2 molecules on the Ti-decorated GO at 298 K and 10 bar using GCMC method (The red points are the centers-of-mass of the adsorbed CO_2 molecules). CO_2 molecules mostly distribute on the GO surface instead of Ti atoms.

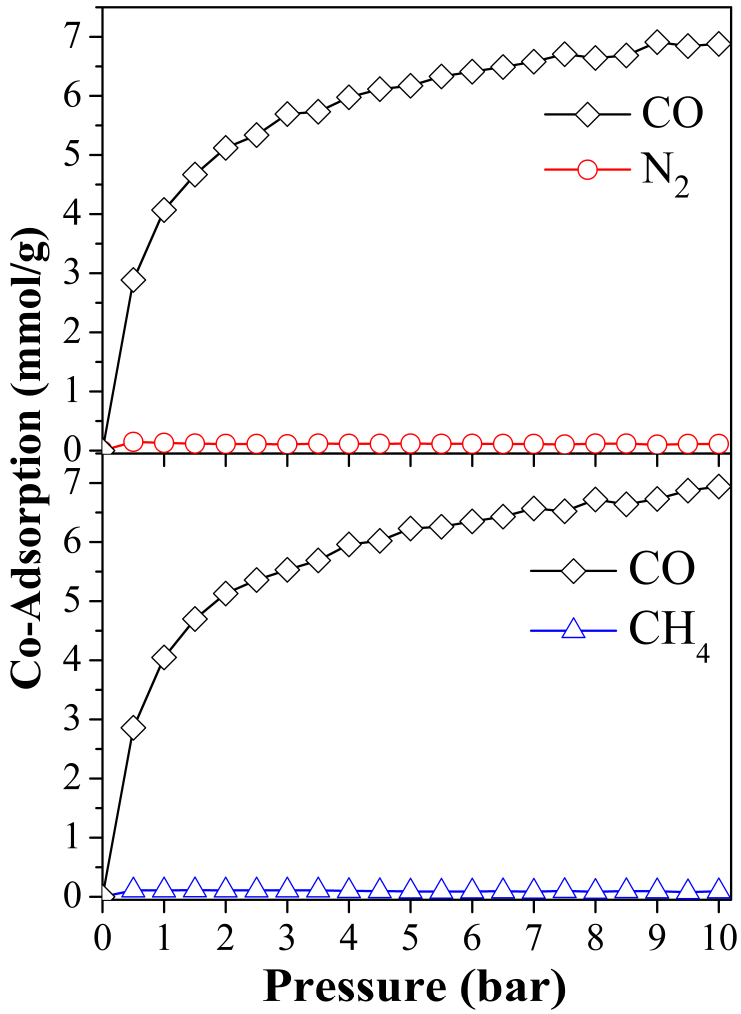

Fig. S2 Co-adsorption isotherms of CO/N_2 and CO/CH_4 gas mixtures at the temperature of 298 K from 0 to 10 bar.