Supporting information

Understanding Adsorption of CO_2, N_2, CH_4 and its Mixture in Functionalized Carbon Nanopipe Array

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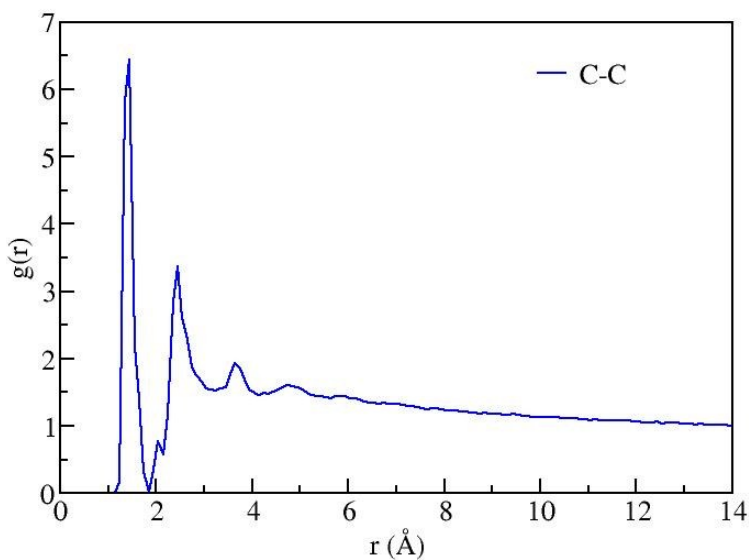
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Supporting information S1:

Radial distribution function of C-C atom in the CMK-5 material are given below,

Supporting information S2:

The chemical potential of reservoir gas, μ, is connected through pressure as

$$\beta\mu = \beta\mu^0_{id.gas} + \ln\left(\beta p_{id.gas}\right)$$

where $p_{id.gas}$ is the pressure of the reservoir assuming ideal gas.

$\mu^0_{id.gas}$ and β are the reference chemical potential and $1/k_BT$, respectively.

List of chemical potentials used in the simulation and the corresponding pressure based on the above relation.

Chemical potential ($\beta\mu$) kcal/mol	Pressure (bar)
-11.0	0.70
-10.5	1.15
-10.0	1.89
-9.5	3.13
-9.0	5.16
-8.5	8.51
-8.0	14.03
-7.8	17.13
-7.5	23.13
-7.0	38.13

Supporting information S3:
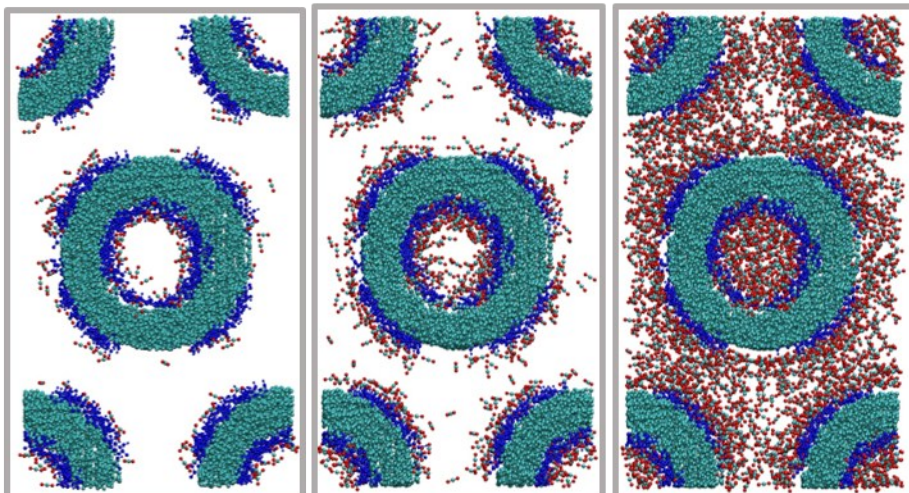
Simulation snapshot of adsorbed gases at different reservoir pressures.
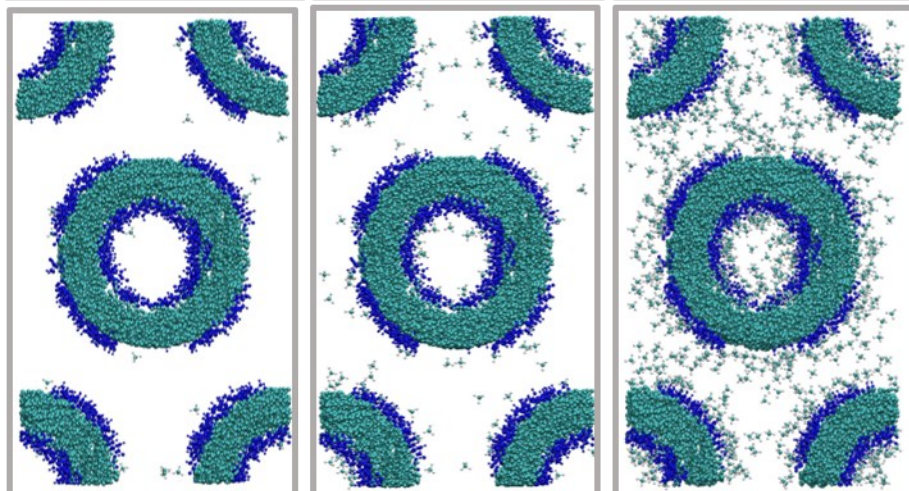
P = 0.7 bar   P = 5.16 bar   P = 38.13 bar

CO_2

CH_4

N_2