MSc in Environmental Engineering

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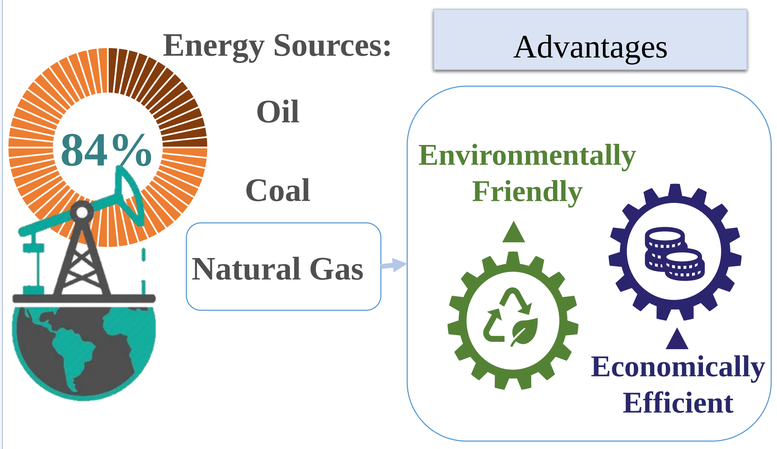
Qatari Tight Gas Reservoirs: Molecular Simulation Insights Toward the Estimation of Ultimate Recovery (EUR) from Carbonated Reservoirs

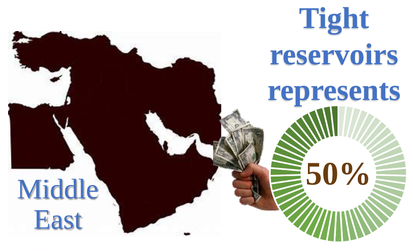
ABSTRACT

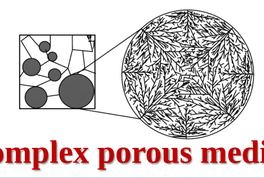
The geometrical properties of the reservoir rocks are usually affected by natural thermodynamics or environmental changes that may affect the amount of gas in place in the reservoir. To address these properties, we conduct DFT calculations to study the effect of gas composition on the gas adsorption, including, **surface strain** and **curvature effects**. Additional analysis like geometrical analysis, and surface energy were conducted and calculated to explain the results. These findings can be useful for determining the estimated ultimate recovery in carbonaceous tight gas reservoirs.

Introduction & Objectives



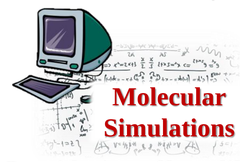
Research problem





Objective

Analyze Gas – Surface Interactions By:



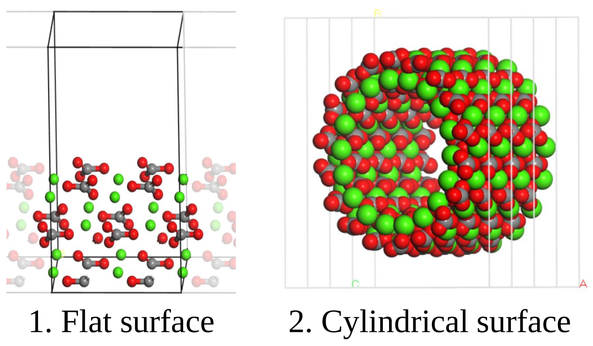
Considering effects like:

a. Surface strain

b. Curvature & Nanopore diameter

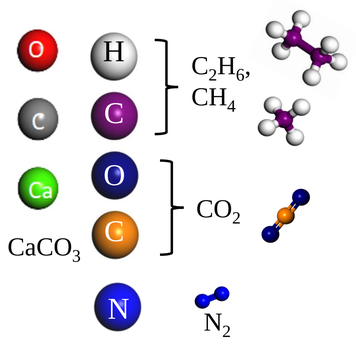
Methodology

a. Creating the model of the porous media by Material Studio

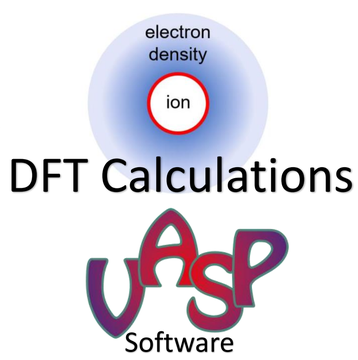


1. Flat surface 2. Cylindrical surface

b. Addition of gas molecules (Color codes):



c. Employ molecular simulations



c. Analysis & Equations

Geometrical Analysis & Surface Energy (γ)

$$\gamma = \frac{(E_{SURF} - nE_{bulk})}{(A_{inner} + A_{outer})} \quad (1)$$

Adsorption Energy (E_{ads}) & Capacity Test

$$E_{ads} = \frac{E_{SURF+NX} - E_{SURF} - (N \times E_X)}{N} \quad (2)$$

Results & Discussions

a. Strain Effect

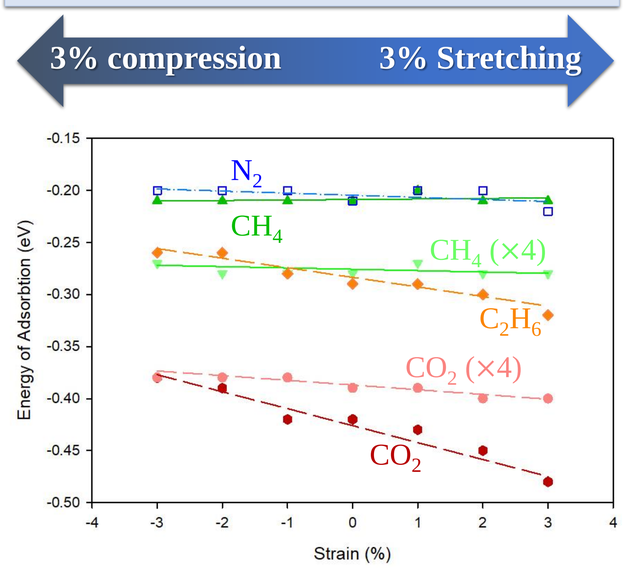


Figure 1: E_{ads} of different gases on strained surfaces.

b. Surface Energy

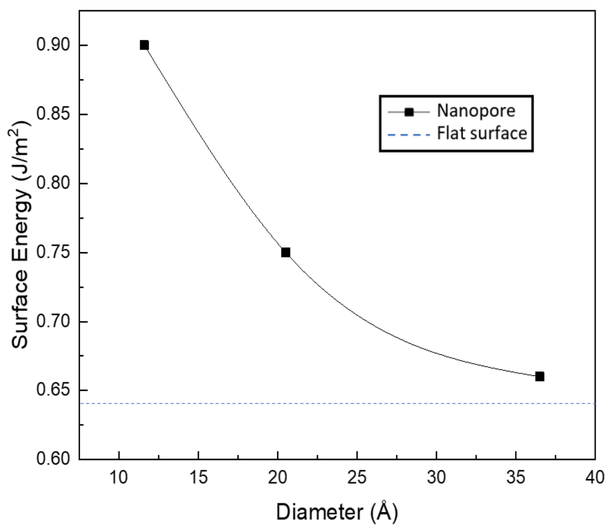
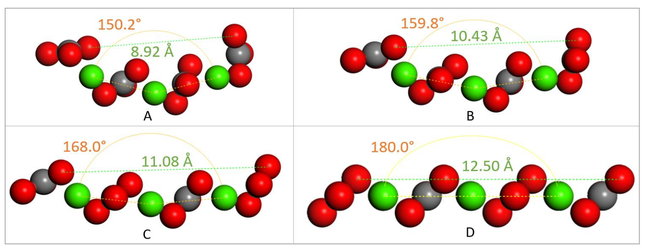


Figure 2: surface energy showing an increase with decreasing the curvature effect.

c. Geometrical Analysis

Table 1: The geometric properties of the nanopores and the flat surface.

	Diameter (nm)	Ca1-Ca2-Ca3 (°)	O1-O4 (Å)
P1	1.16	150.2	8.92
P2	2.05	159.8	10.43
P3	3.56	168.0	11.08
Flat surface	-	180.0	12.50



d. Capacity Test

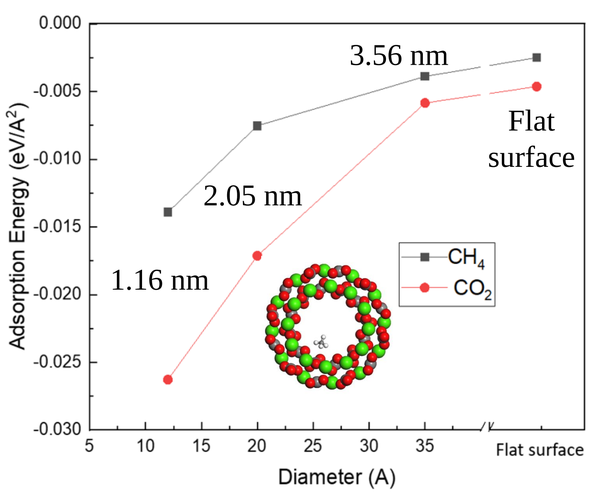


Figure 3: E_{ads} of the three nanopores and the flat surface.

Developed mathematical model:

$$CH_4: Ln[-E_{ads}] = -5.106 - 0.066 \times D \quad R^2 = 0.995 \ (3)$$

$$CO_2: Ln[-E_{ads}] = -6.002 - 0.054 \times D \quad R^2 = 0.977 \ (4)$$

e. Capacity Test

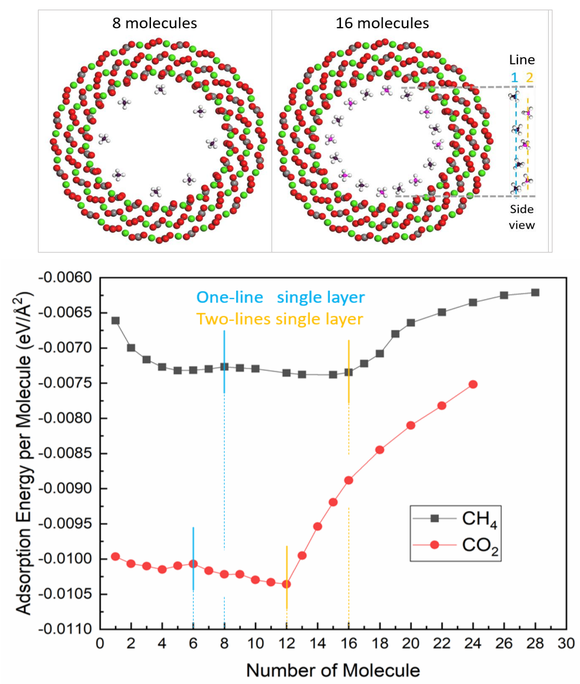


Figure 4: Capacity test for adsorption energy of CH_4 and CO_2 per molecule.

Conclusions

- All the studied gases were physiosorbed to the surface, with CO_2 having higher adsorption energy in all cases.
- The affinity of specific gases to the surface increases with stretching, and the result differ with gases conc.
- Curved nanopore surfaces have more surface energy and different geometrical properties resulting in higher gas adsorption affinity compared to the flat surface.
- The cylindrical nanopore absorbed more than 24 molecules of both CH_4 and CO_2 with alteration of E_{ads} with formation of new layers.
- Three papers are published as outcomes of this work.

References

1. **E. Elbashier**, I. Hussein, G. Carchini, A. Sakhaee Pour, G.R. Berdiyorov, Effect of strain on gas adsorption in tight gas carbonates: A DFT study, Comput. Mater. Sci. (2020) 110186.
2. **E. Elbashier**, I. Hussein, G. Carchini, A. Kasha, G. Berdiyorov. Influence of natural gas composition on adsorption in calcite Nanopores: A DFT study. Applied Surface Science, Volume 568 (2021) 150940.
3. G.R. Berdiyorov, **E. Elbashier**, G. Carchini, I.A. Hussein, A. Sakhaee-Pour. The effect of vacancy defects on the adsorption of methane on calcite 104 surface, Journal of Materials Research and Technology. (2021) ISSN 2238-7854.