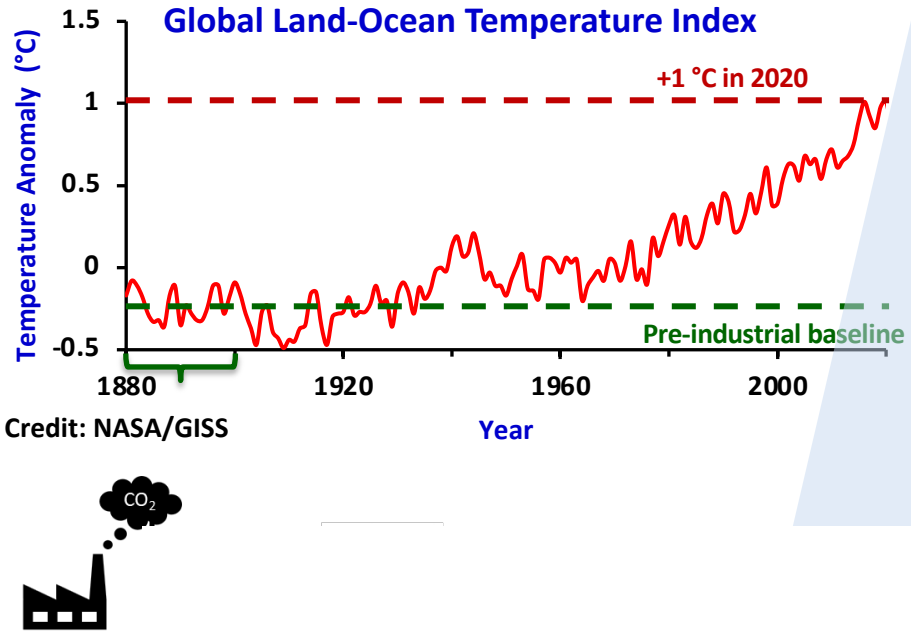
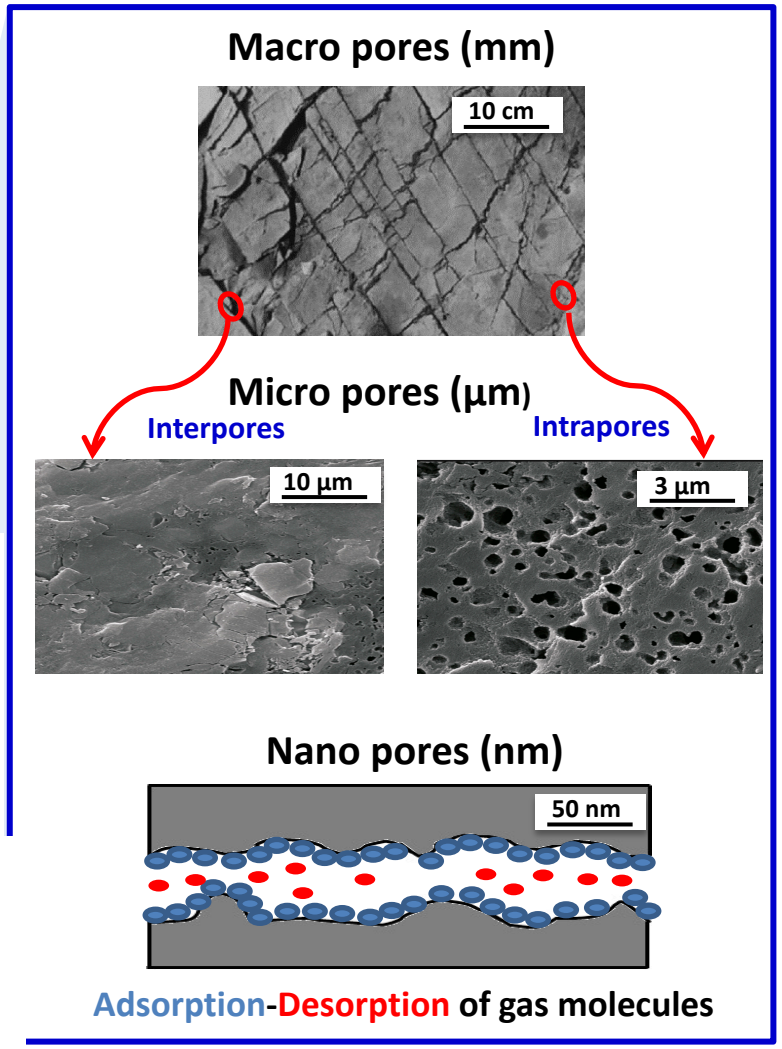
Impacts of Geochemistry on Carbon Dioxide Adsorption in Organic-Rich Mudrocks

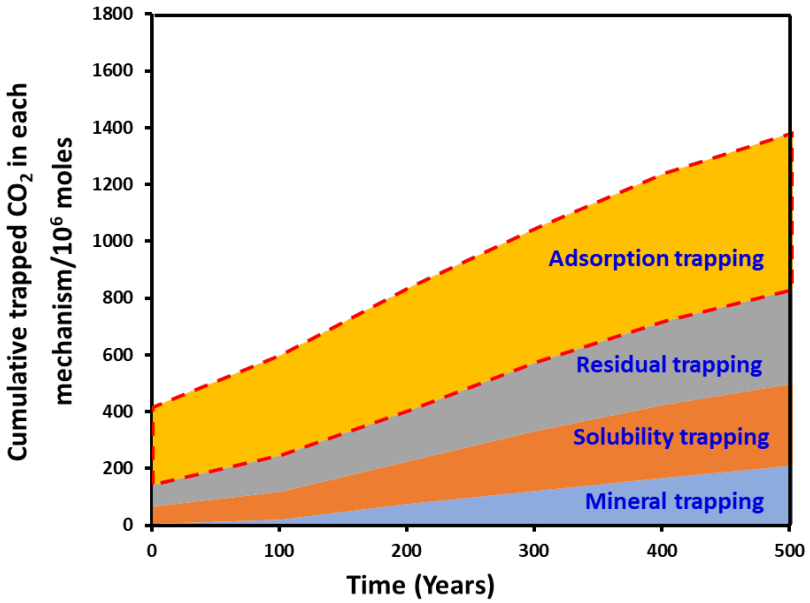
Ibrahim Gomaa, Zoya Heidari, and D. Nicolas Espinoza

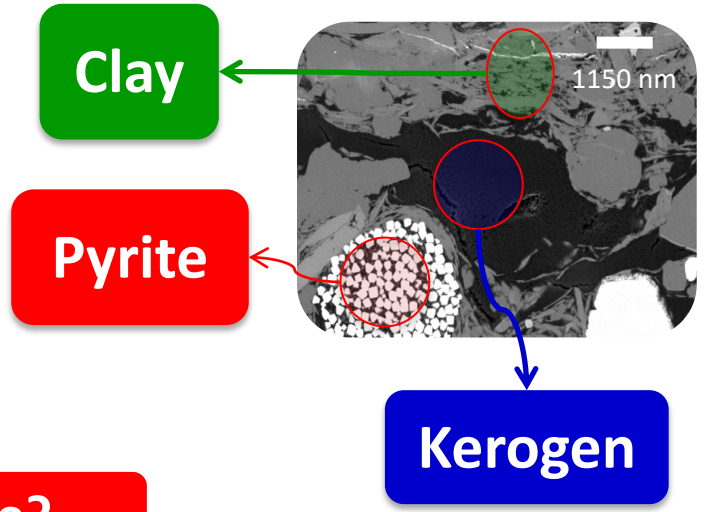
The University of Texas at Austin

Motivation: CO_2 Storage in Organic Shale



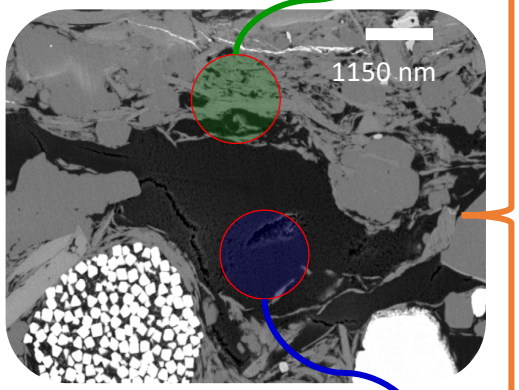






What parameters affect CO_2 adsorption in organic shale?

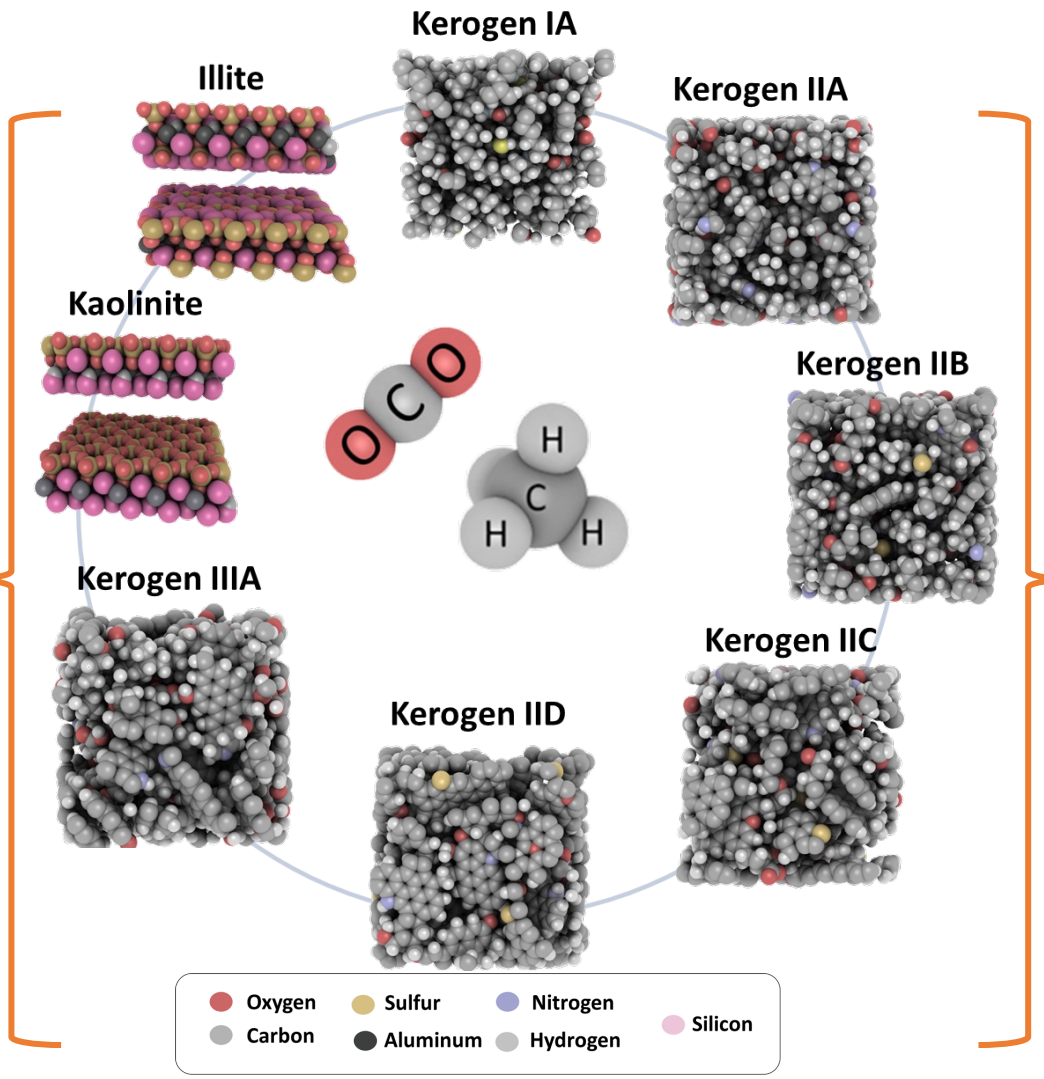
Methods and Modeling: CO_2 Storage in Organic Shale



Clay

Kerogen

Molecular Simulation

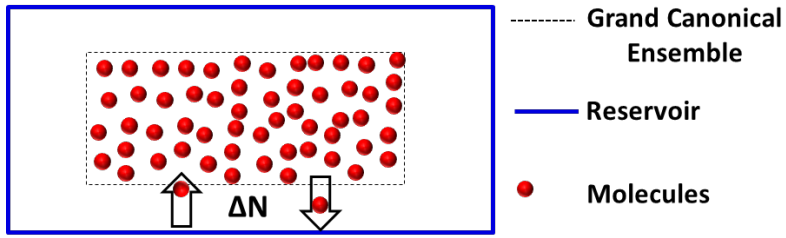


Kerogen IIA | Kerogen IIB | Kerogen IIC | Kerogen IID

Increasing Thermal Maturity

- Illite and Kaolinite clays have the same pore size of 2 nm.
- Illite clay surface has a net negative charge.

Grand Canonical Monte Carlo (GCMC) simulations

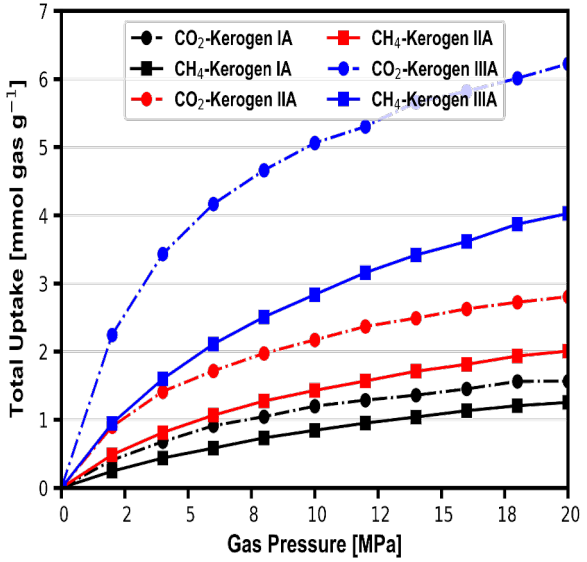


System Total Energy

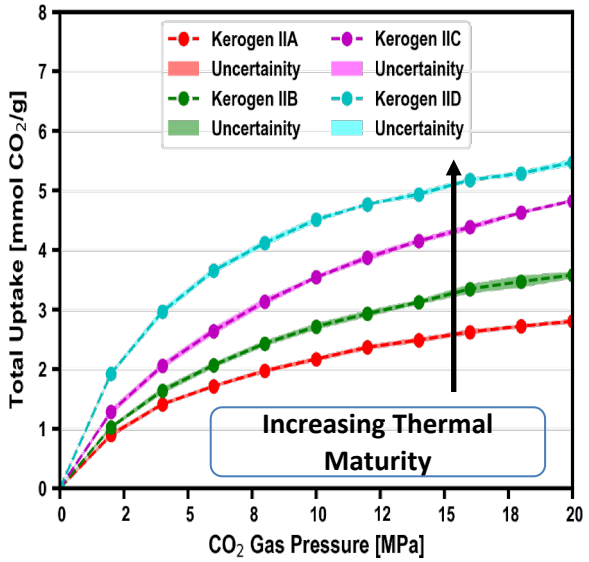
$$U = \sum 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] + \sum \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}$$

Results: CO_2 Storage in Organic Shale

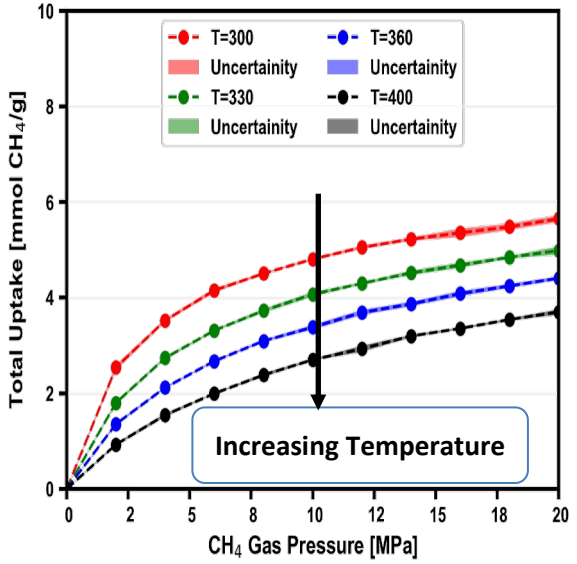
Influence of Kerogen Types on CO_2 – CH_4 Sorption



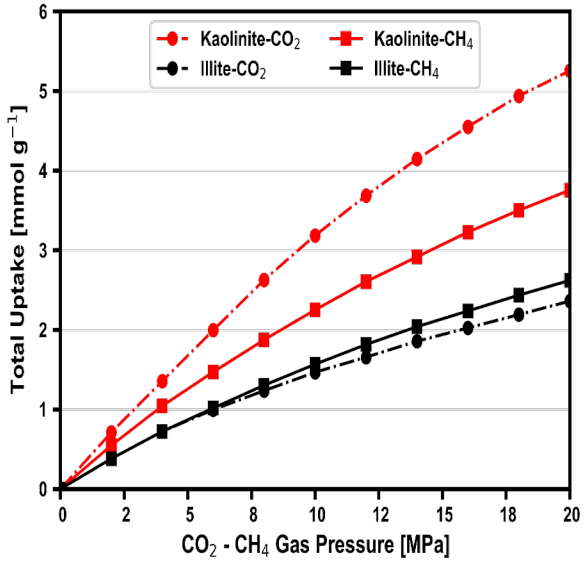
Influence of Kerogen Thermal Maturity on CO_2 Sorption

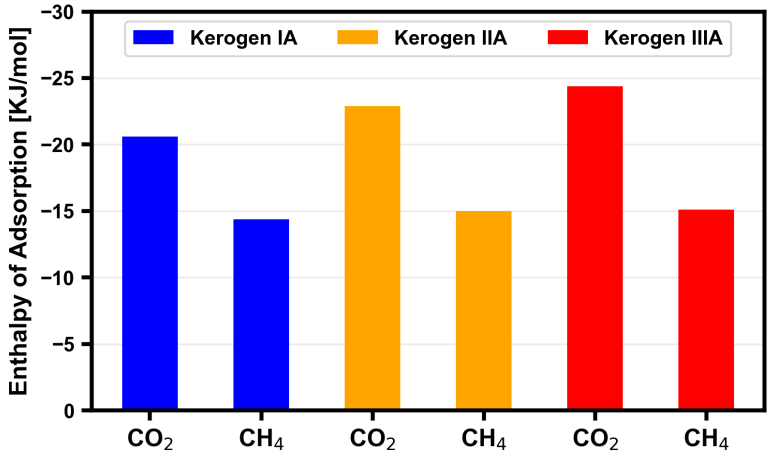


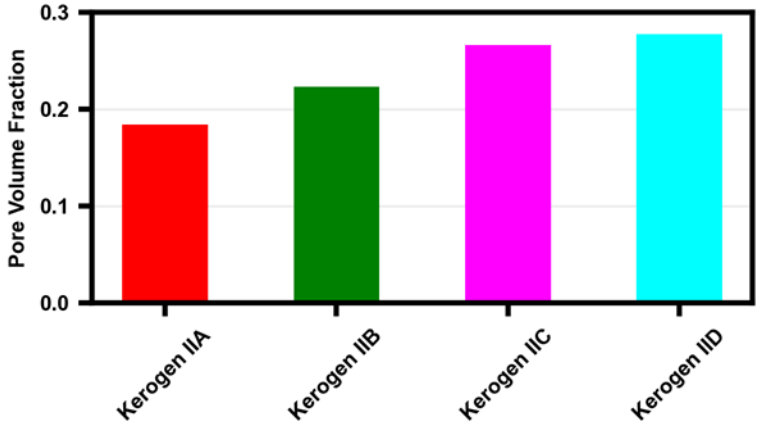
Influence of Reservoir Temperature on CO_2 Sorption

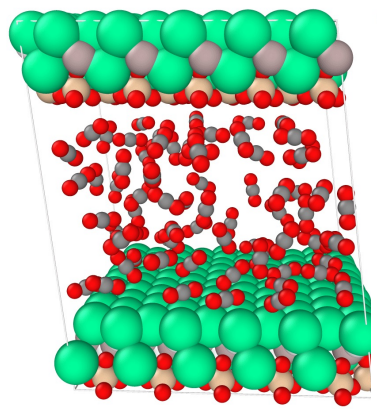


CO_2 – CH_4 Competitive Sorption on Clay Surfaces

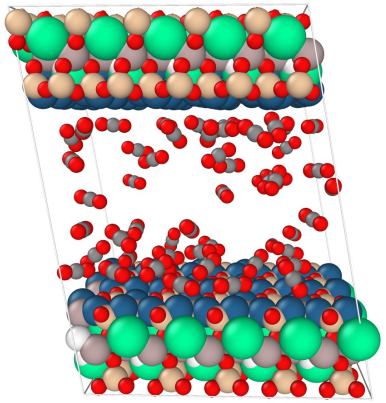








Kaolinite



Illite

Impacts of Geochemistry on Carbon Dioxide Adsorption in Organic-Rich Mudrocks

Ibrahim Gomaa, Zoya Heidari, and D. Nicolas Espinoza
The University of Texas at Austin