



Office of Science



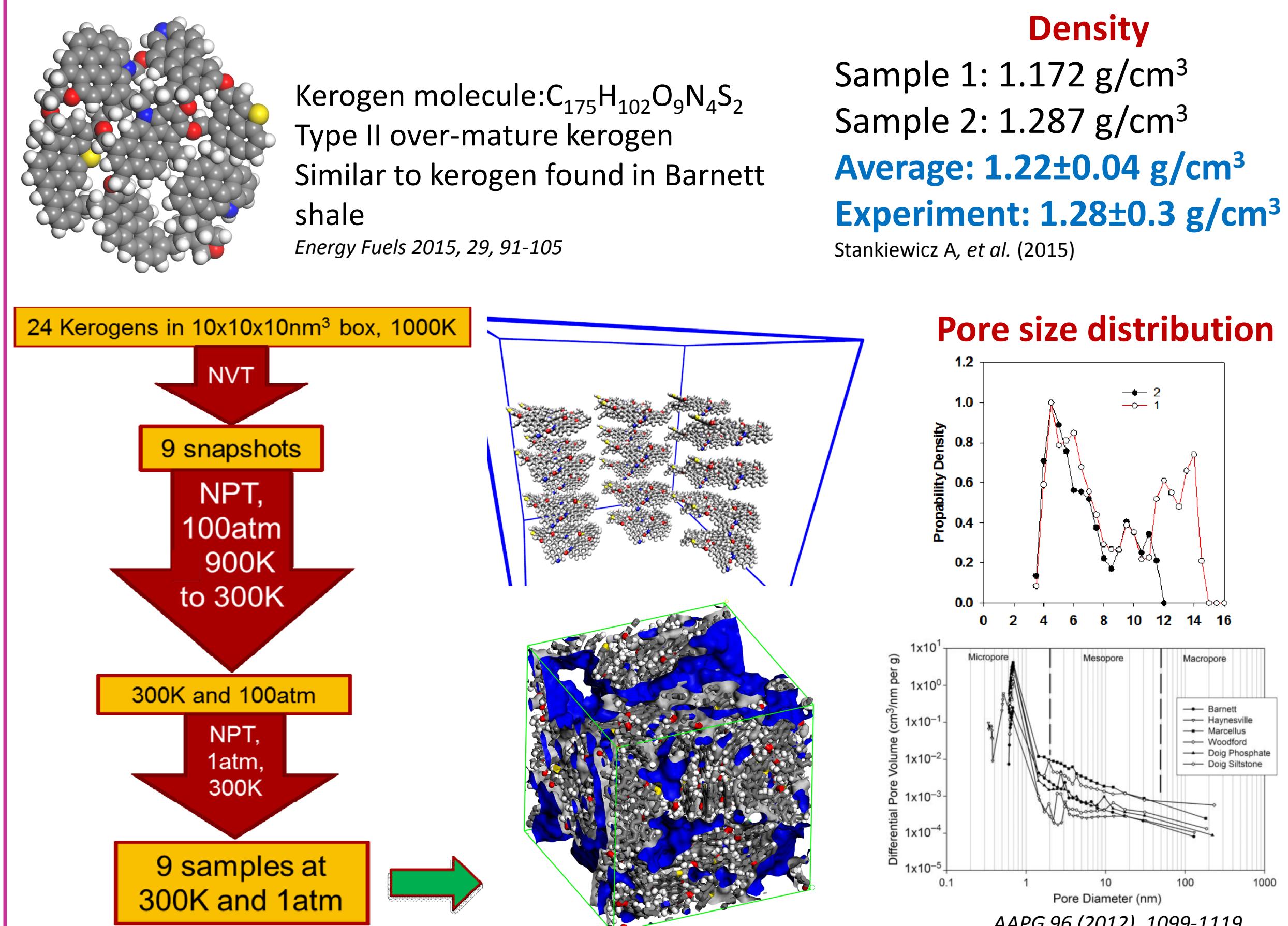
# Differential retention and release of $\text{CO}_2$ and $\text{CH}_4$ in kerogen nanopores from molecular simulations

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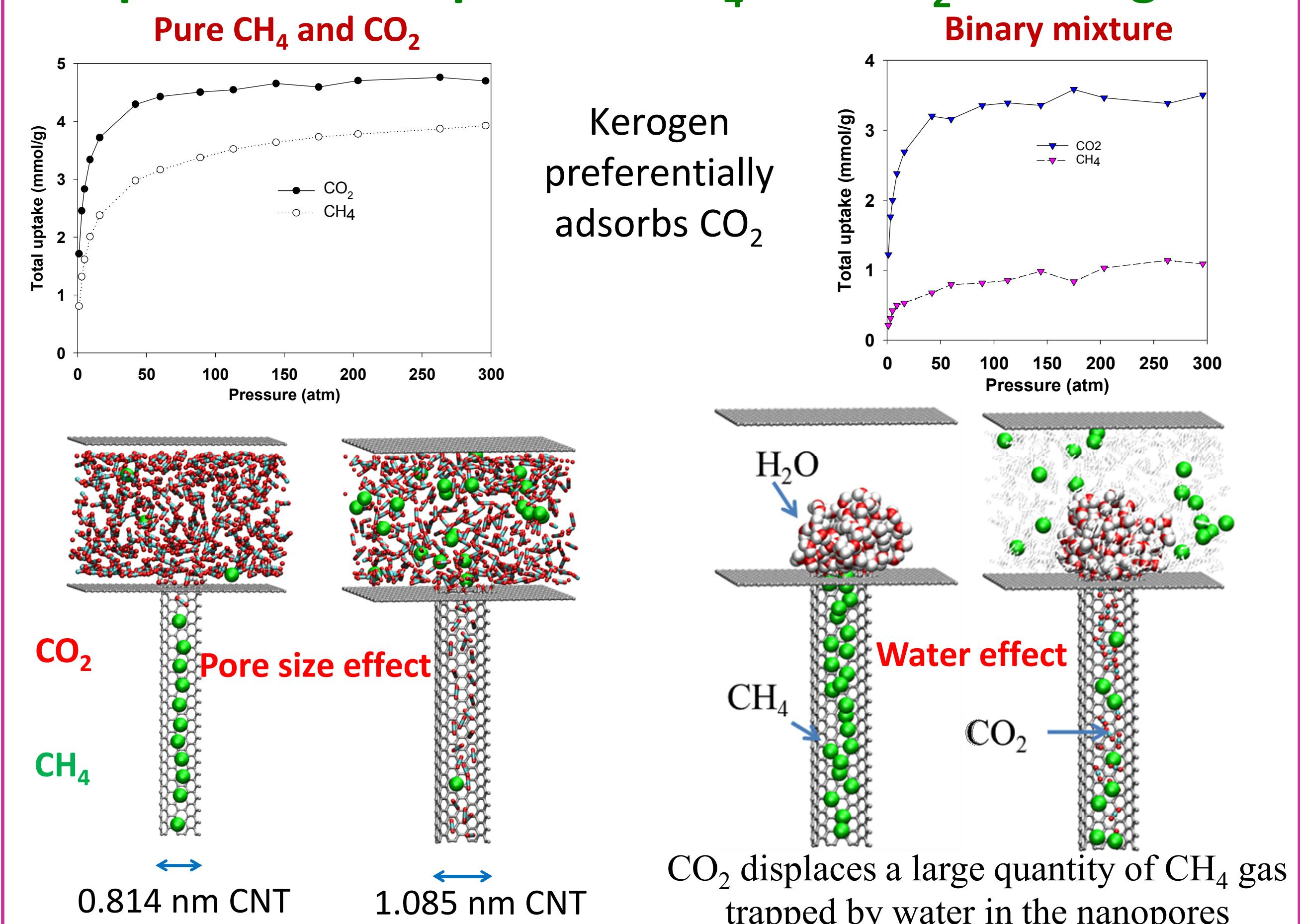
## Objective

Understanding nano-structural properties of subsurface porous media including kerogen and clay, and gas adsorption and transport in subsurface porous media.

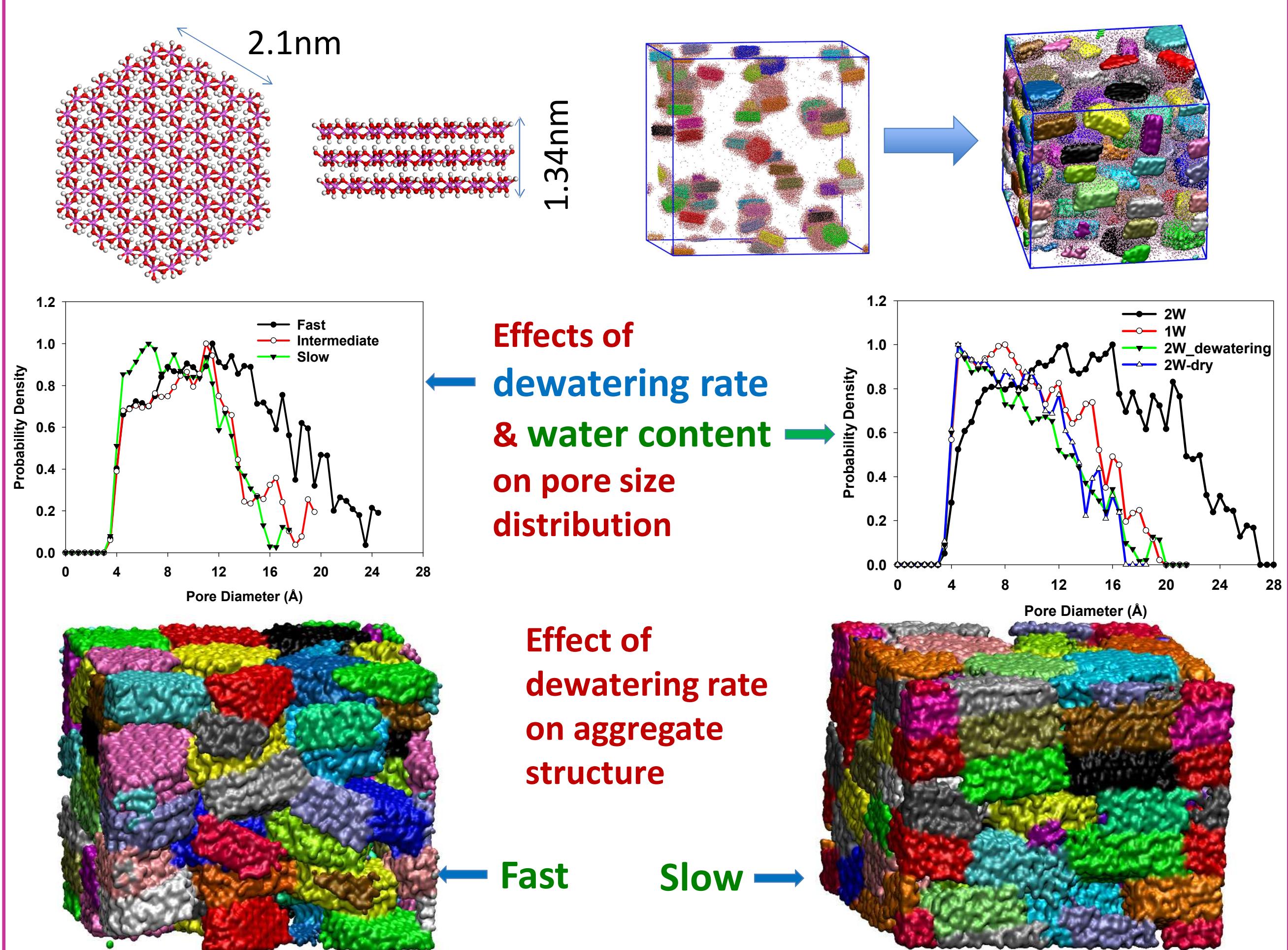
## Formation of condensed kerogen



## Competitive adsorption of $\text{CH}_4$ and $\text{CO}_2$ in kerogen



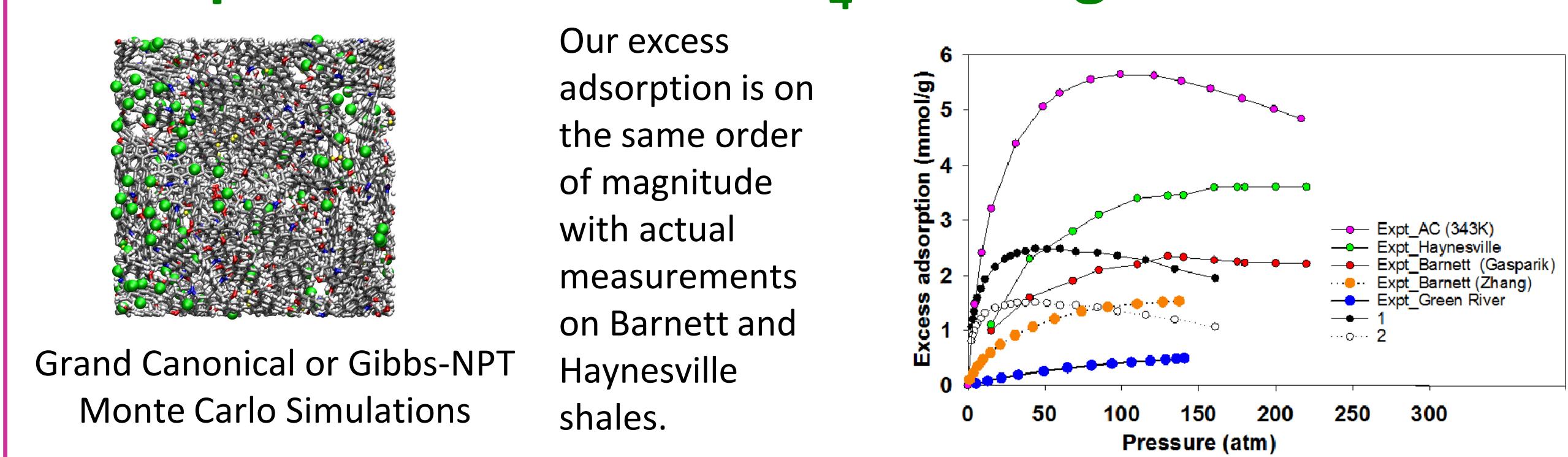
## Nano-structural properties of clay aggregates



## Conclusions

- Methane release from kerogen matrix is characterized by fast release of pressurized free gas followed by slow release of adsorbed gas. A significant amount of gas deposited in kerogen can be trapped in isolated pores and thus not recoverable. (*Sci. Rep.* 6, 28053)
- Kerogen preferentially retains  $\text{CO}_2$  over  $\text{CH}_4$ . When water is present in the kerogen matrix, it may block  $\text{CH}_4$  release. However, the addition of  $\text{CO}_2$  to a matrix may enhance  $\text{CH}_4$  release because  $\text{CO}_2$  can migrate through water and exchange for adsorbed methane.
- Dewatering and water content affect micro-porosity of clay aggregates. Slow dewatering will create more compact aggregates compared to fast dewatering. The amount of water present in the clay aggregates strongly affects the particle-particle interactions and hence the clay aggregate structure. (*Sci. Rep.* 7, 15286)

## Adsorption isotherm of $\text{CH}_4$ in kerogen



## Extraction of $\text{CH}_4$ from nanopores in kerogen

