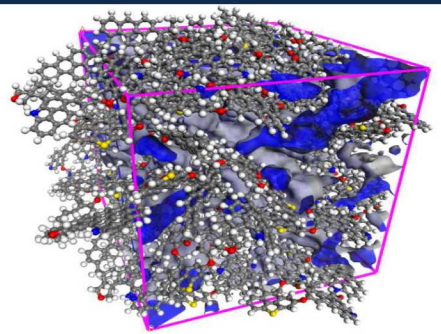
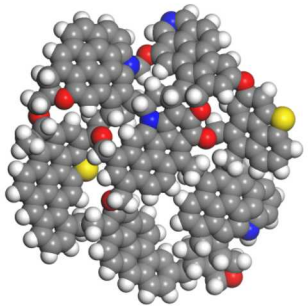
SAND2018-8789C





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BOSTON 2018 | AUGUST 12-17

Molecular Modeling of Interaction between Kerogen and Pore Fluid

Tuan A. Ho, Yifeng Wang, Louise J. Criscenti
Sandia National Laboratories

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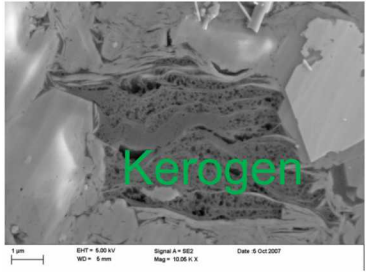
Introduction

Kerogen

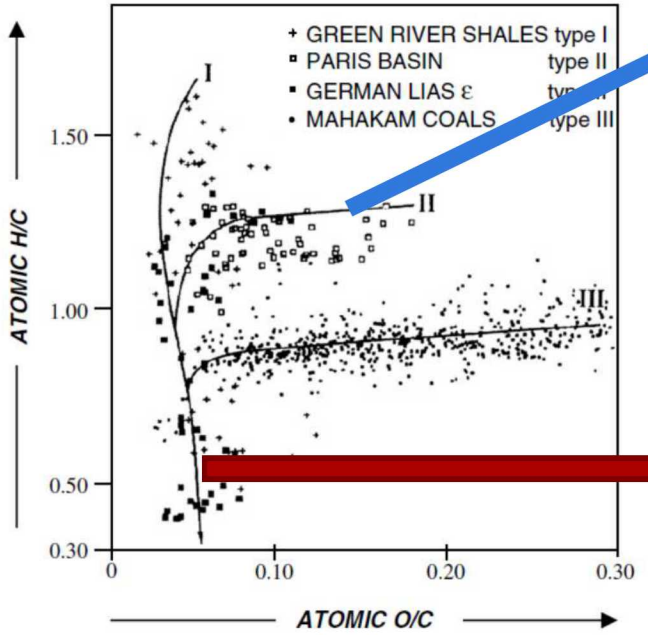


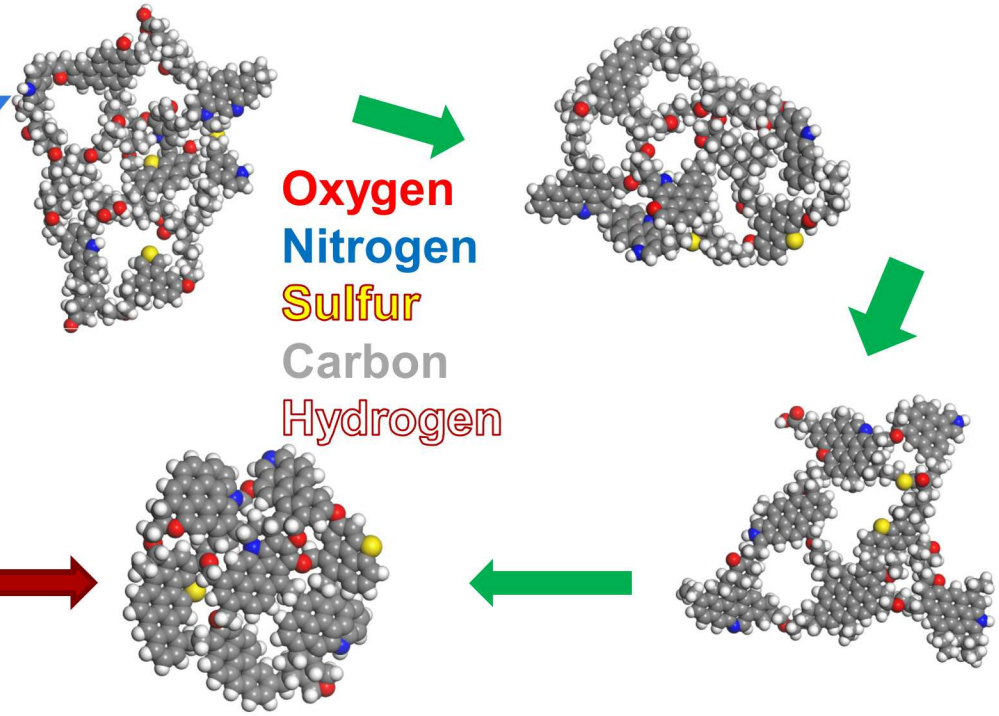
- Insoluble organic matter found in sedimentary rocks (geochemistry)

- Cracks into petroleum products (kerogen maturation, petroleum generation)

  Van Krevelen diagram

Organic Geochemistry 38, 719-833 (2007)





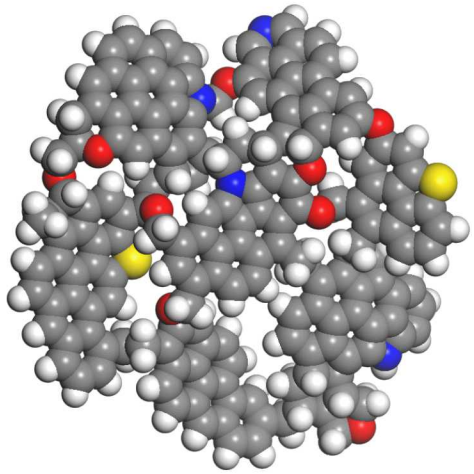
Ungerer et al., Energ Fuel 29, 91-105

- **Hosts pore space responsible for petroleum storage and transport**

Overmature Kerogen

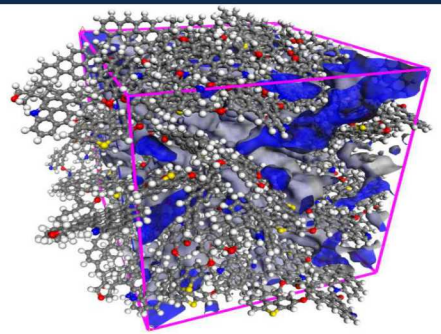
- Use the available elemental analysis and functional data from XPS and ^{13}C NMR
  - *(Energy & Fuels, 2007, 21, 1548-1561)*

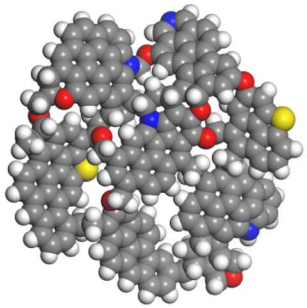
Oxygen
Nitrogen
Sulfur
Carbon
Hydrogen



	II-D	
	analytical data	model unit
H/C	0.56	0.58
O/C	0.047	0.051
N/C	0.021	0.023
S/C	0.01	0.011
% of aromatic carbon from XPS(a) or NMR(b)	72(a), 80(b)	79
avg. number of C atoms per aromatic cluster	20	19.9
fraction of aromatic carbons with attachments (sp^3 C, N, S, O)	0.24	0.28

Molecular Modeling of Interaction between Kerogen and Pore Fluid





Outline:

1. **Nanostructure of kerogen**
2. **CH_4/CO_2 adsorption onto kerogen**
3. **Kerogen swelling**

Formation of condensed kerogen

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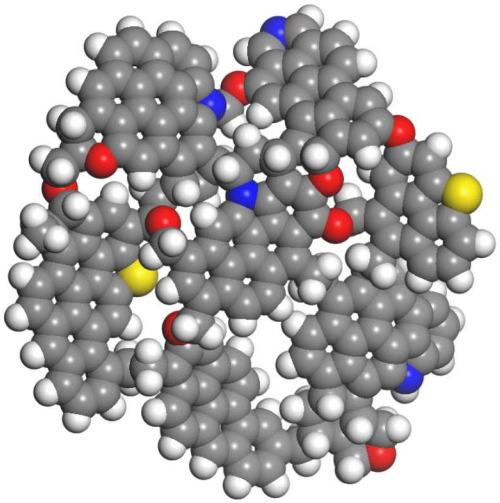


$C_{175}H_{102}O_9N_4S_2$

Energy Fuels 2015, 29, 91-105

24 Kerogens in 10x10x10nm^3 box, 1000K

NVT

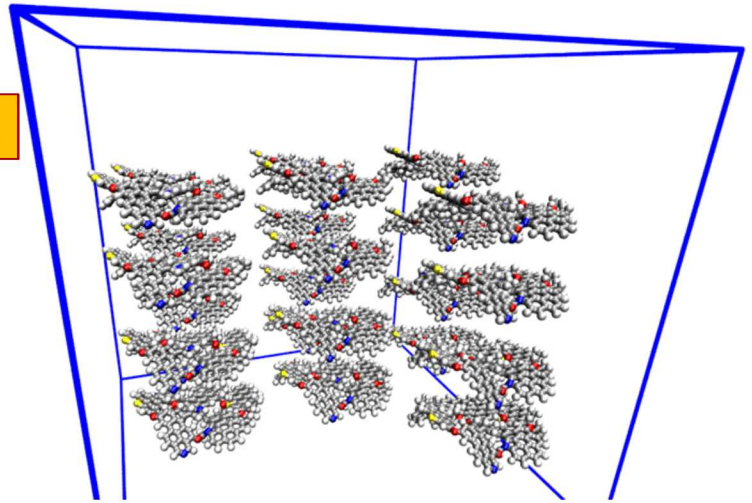
9 snapshots

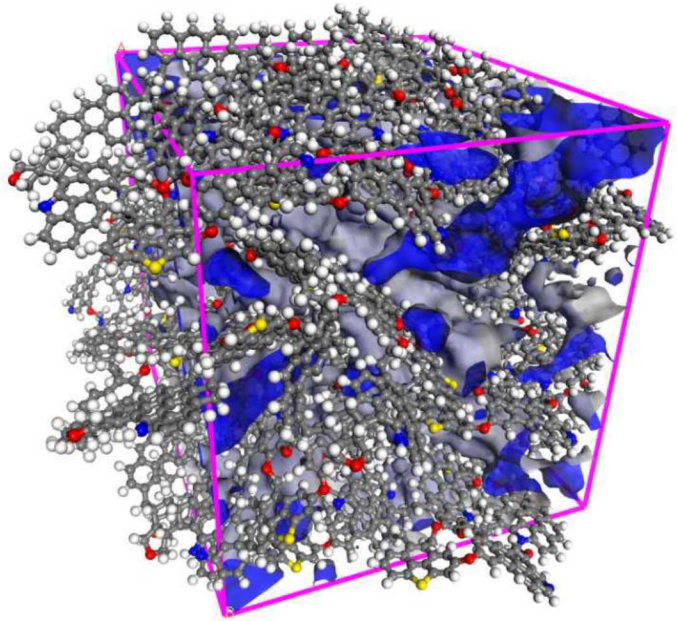
NPT, 100at, 900K to 300K

300K and 100atm

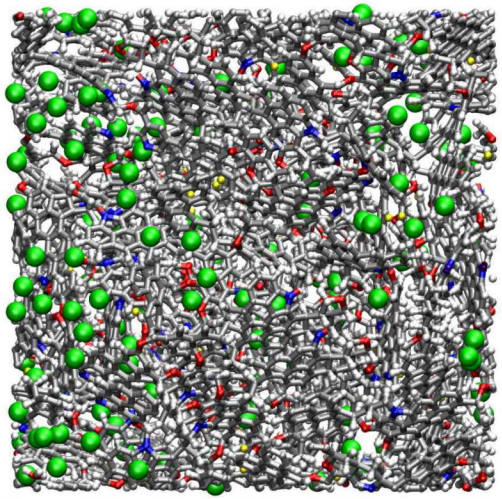
NPT, 1atm, 300K

9 samples at 300K and 1atm





Characterization



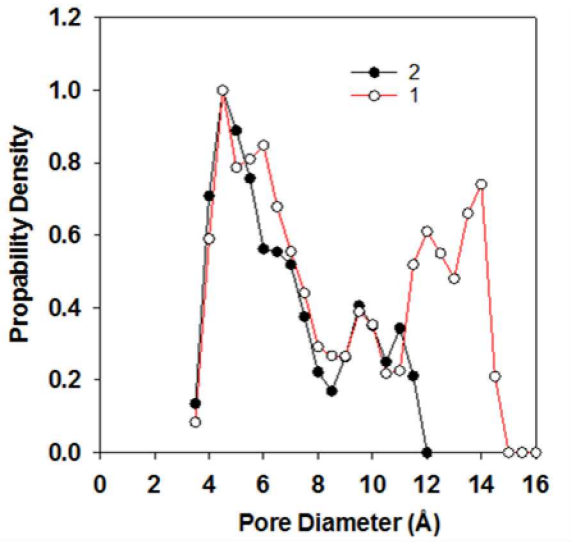
Density

Average :1.22±0.04 g/cm^3

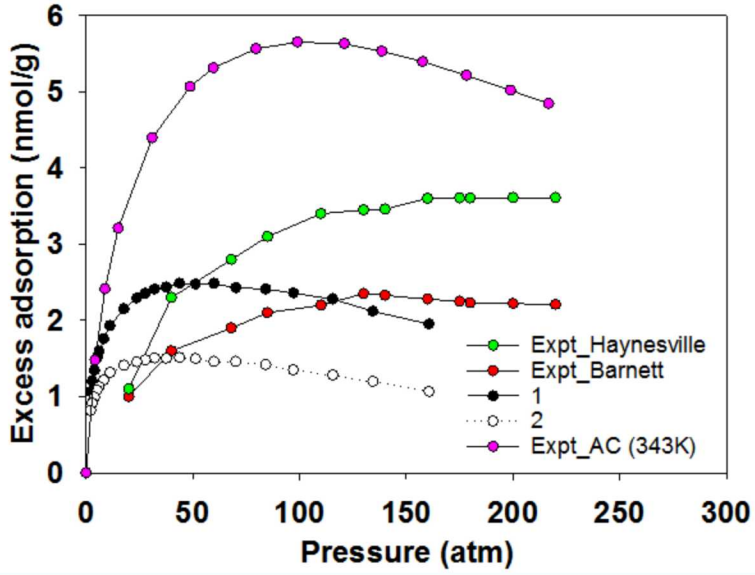
Experiment: 1.28±0.3g/cm^3

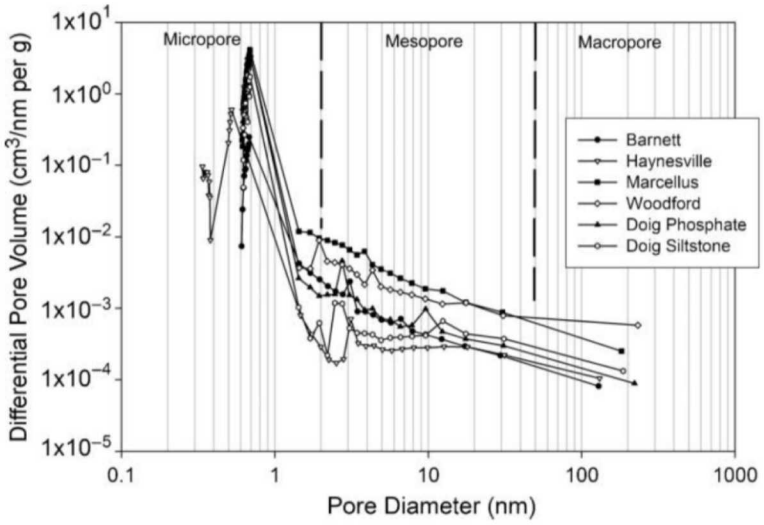
Stankiewicz A, *et al.* (2015) Kerogen density revisited – lessons from the Duvernay Shale. *In: Paper URTeC 2157904 at the Unconventional Resources Technology Conference, San Antonio, Texas, July 2015*

Pore size distribution



CH_4 Adsorption





AAPG 96 (2012), 1099-1119

Methane extraction from kerogen

(Scientific Reports 6, 28053, 2017)

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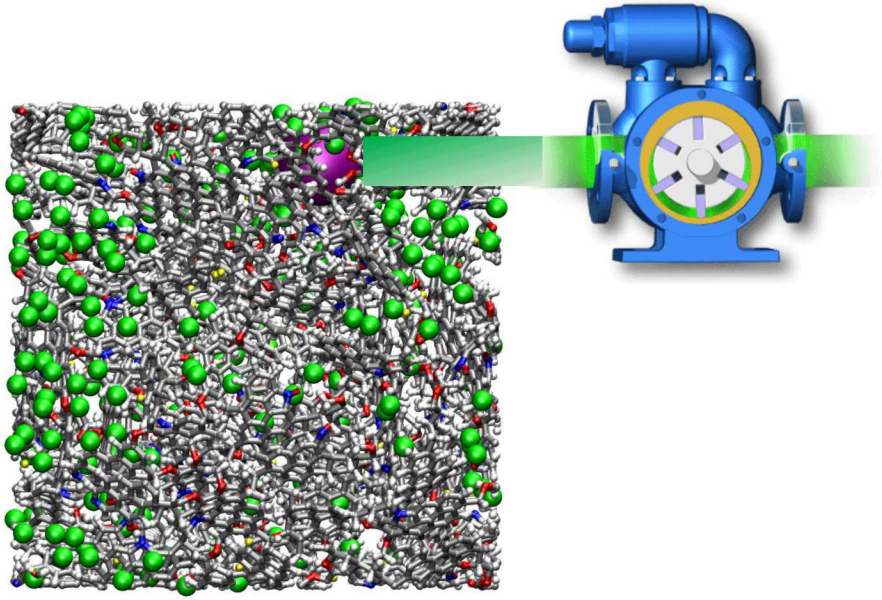
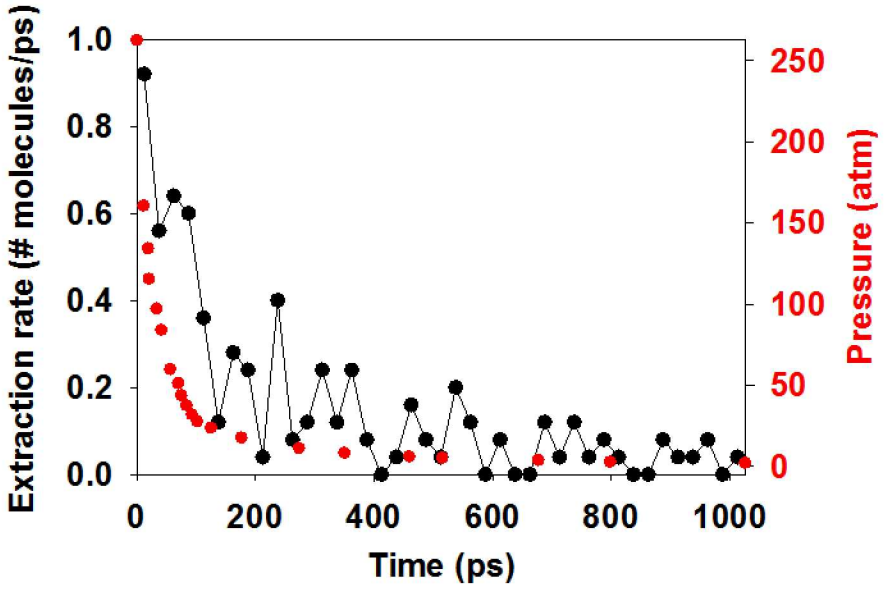
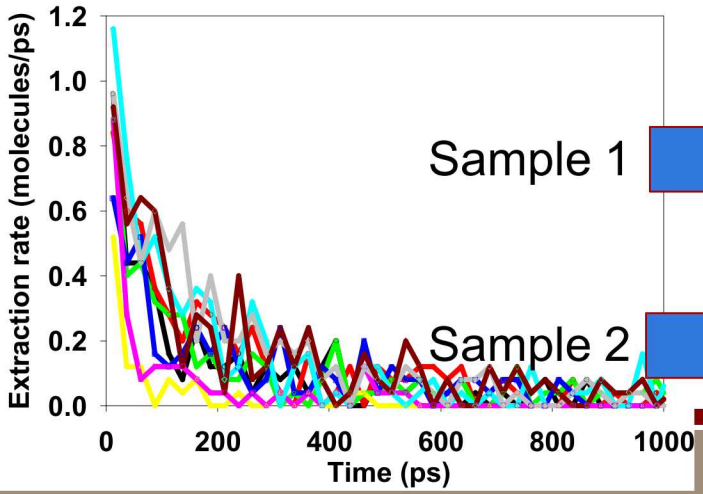
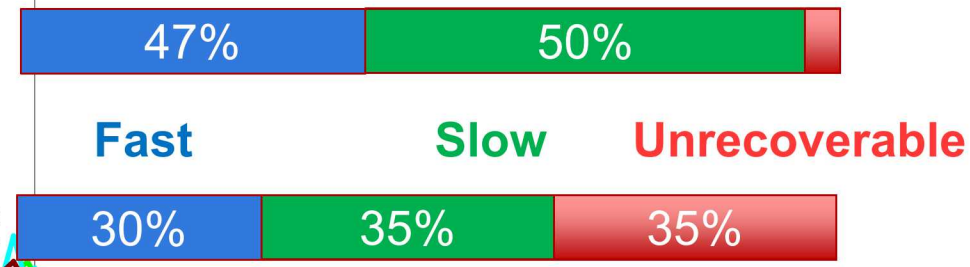
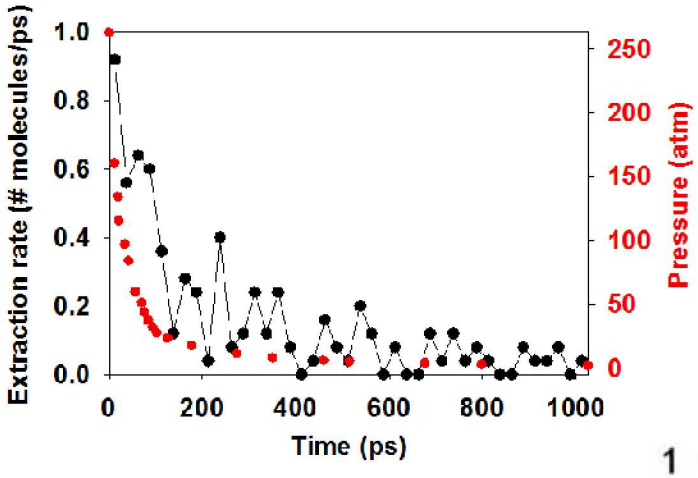


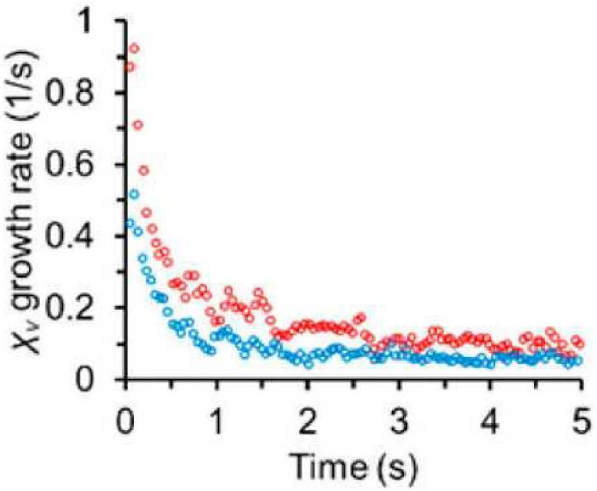




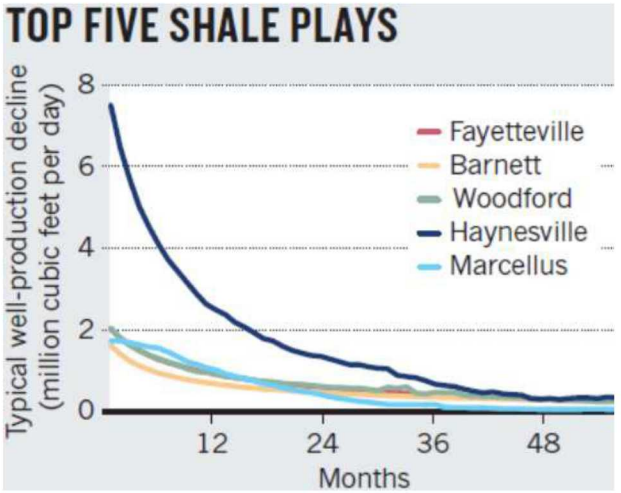


Production decline curve



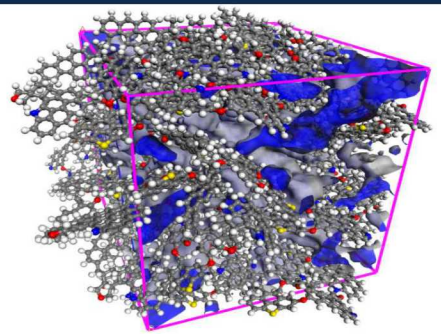


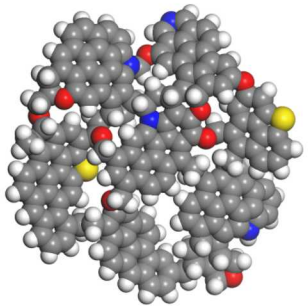
ACS Applied Nano Materials1, 1332-1338 (2018)



Nature 494, 307 (2013)

Molecular Modeling of Interaction between Kerogen and Pore Fluid





Outline:

1. **Nanostructure of kerogen**
2. **CH_4/CO_2 adsorption onto kerogen**
3. **Kerogen swelling**

Differential retention and release of CO_2 and CH_4 in kerogen nanopores (Fuel 220, 1-7, 2018)

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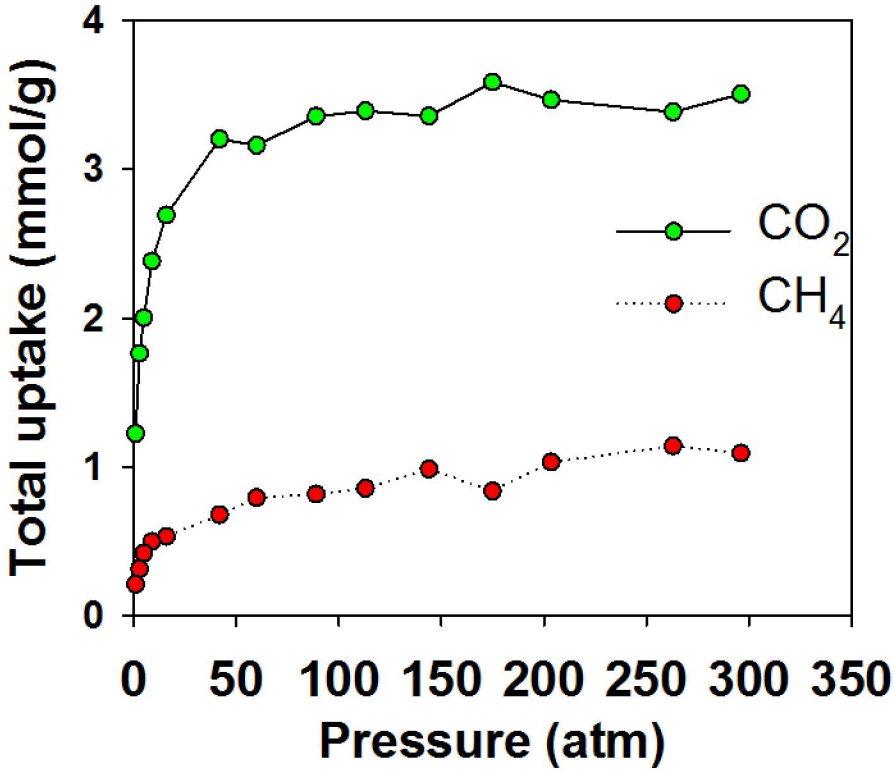
Implications for gas enhanced recovery and carbon sequestration

1:1 binary gas adsorption



Kerogen preferentially retains CO_2 over CH_4

Pore specific effects on enhanced gas recovery

(Fuel 220, 1-7, 2018)

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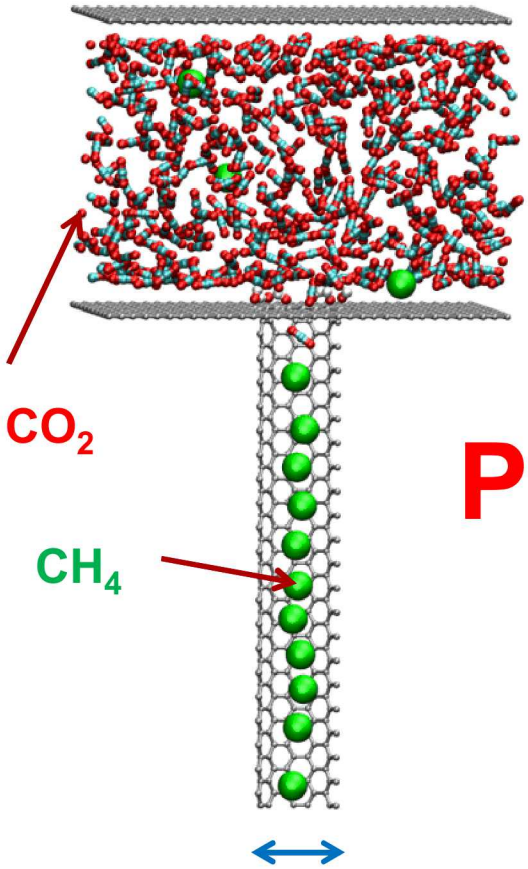
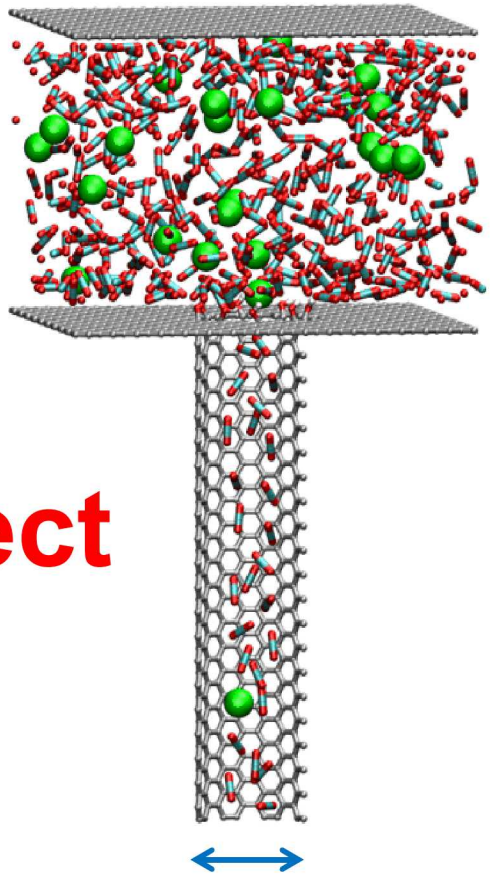


0.814 nm CNT

Pore is too small for the invasion of CO_2

Pore size effect

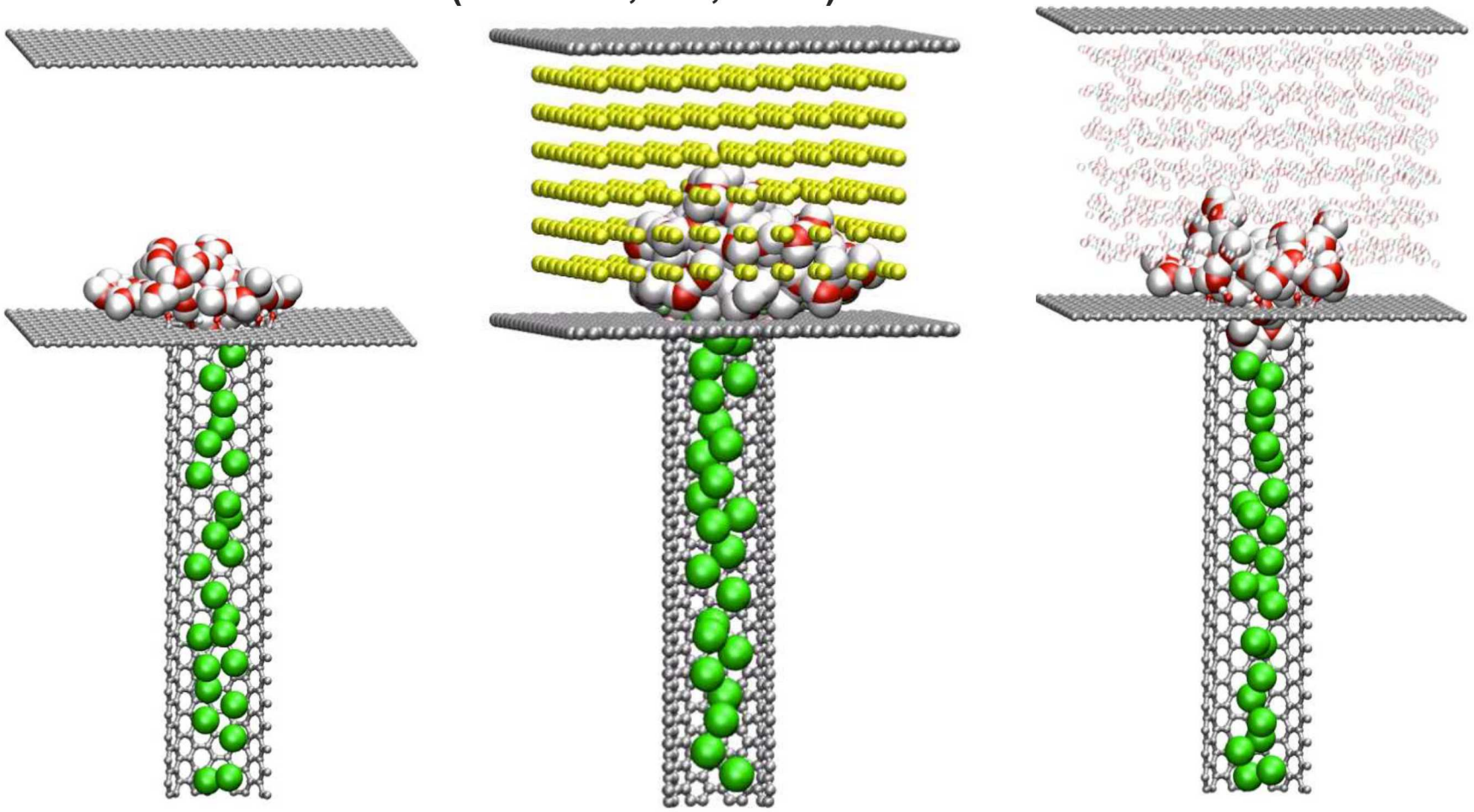


1.085 nm CNT

Pore is big enough for the invasion of CO_2

Pore specific effects on enhanced gas recovery

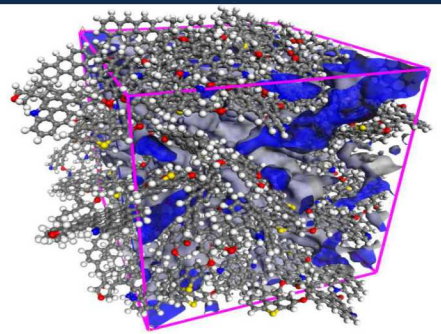
(Fuel 220, 1-7, 2018)

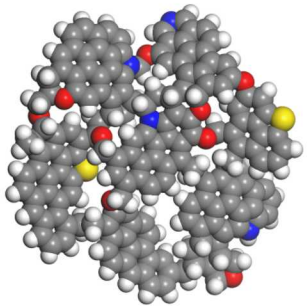


Assume that water drop blocks the pore entrance.

CO_2 invades through water and replaces CH_4 in the nanopore.

Molecular Modeling of Interaction between Kerogen and Pore Fluid





Outline:

1. **Nanostructure of kerogen**
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Kerogen swelling

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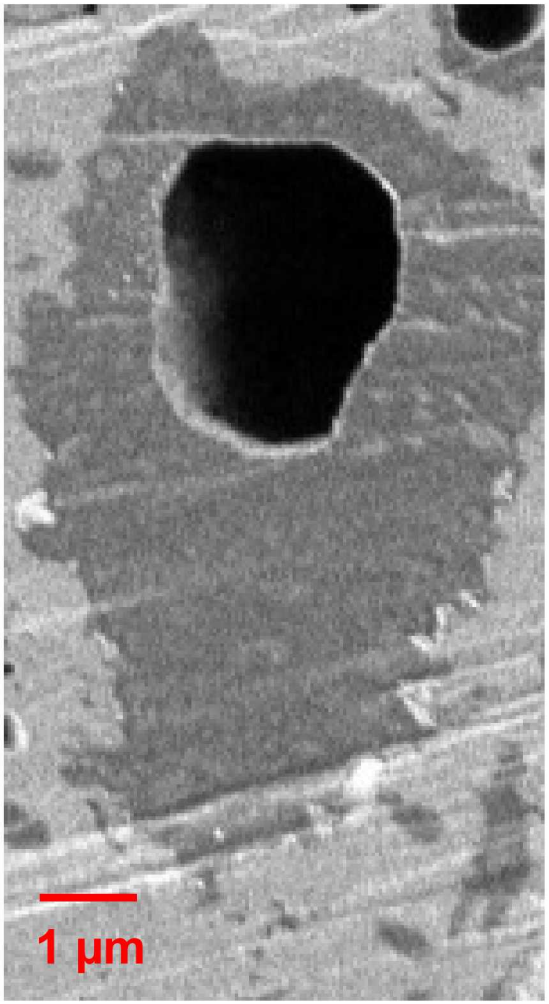
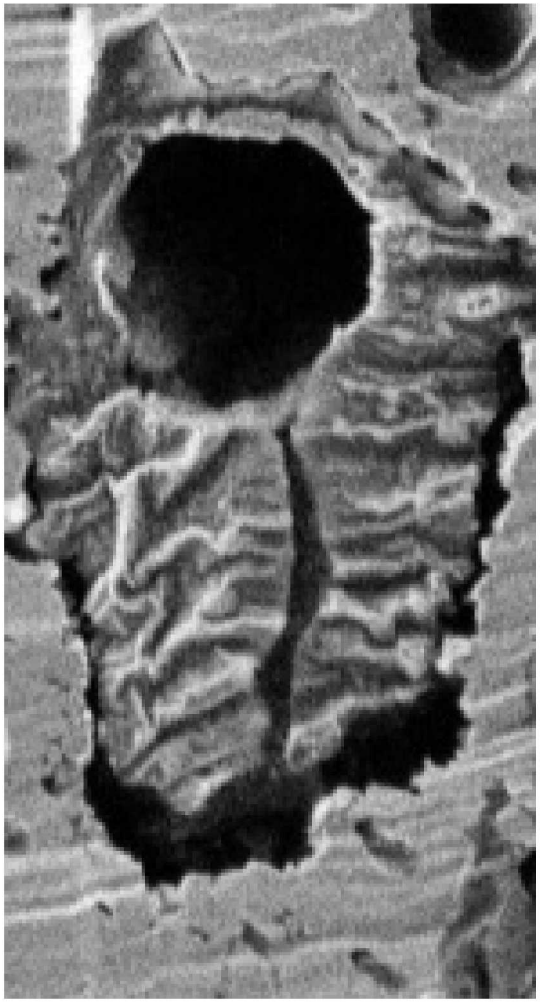
Rubber swelling in oil

From: **Drew Pomerantz**, Schlumberger

Will kerogen swell upon gas adsorption?



Intact shale with swollen kerogen



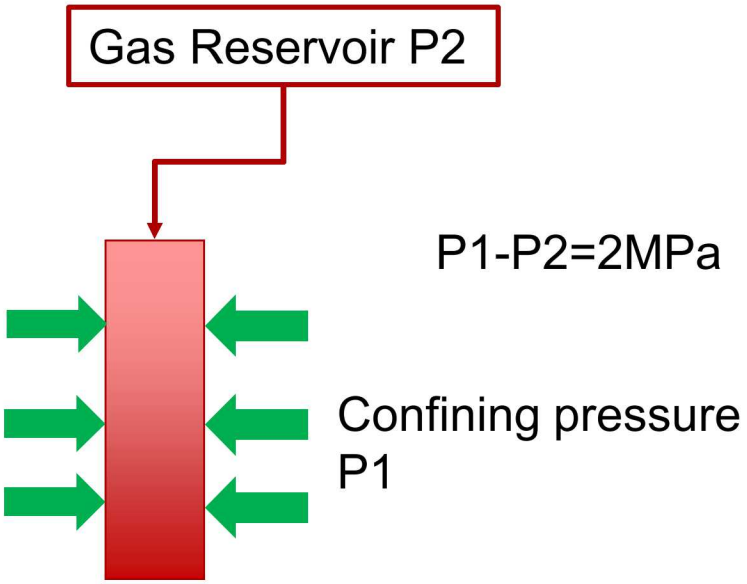
Bitumen-extracted shale with collapsed kerogen

Chemo-mechanical coupling in kerogen gas adsorption (PCCP 20, 11390, 2018)

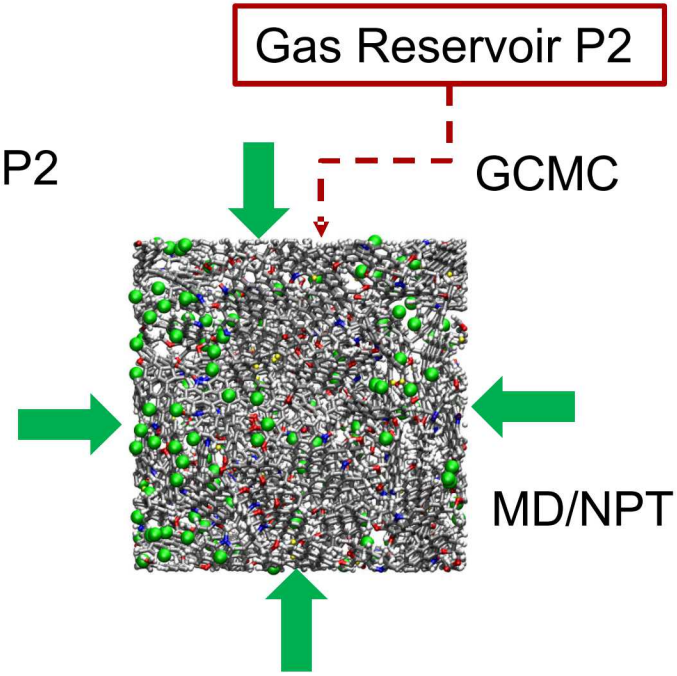
Sandia National Laboratories

Experimental setup

(J. Unconv. Oil Gas Resour., 2014)



Simulation: Hybrid MD/MC

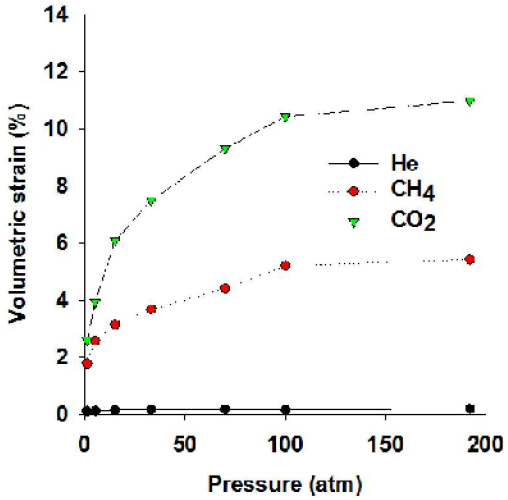


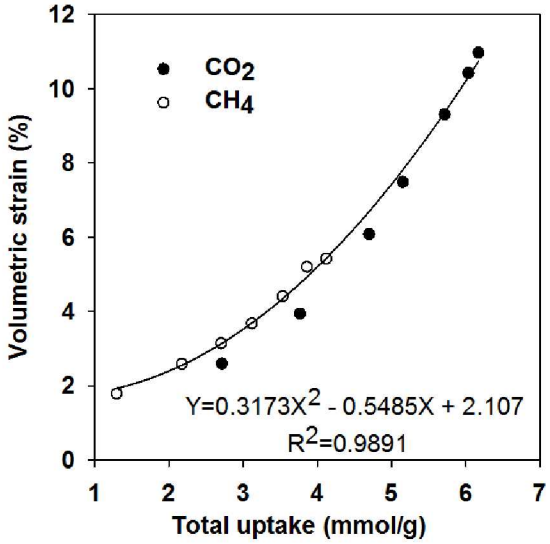
$$Volumetric\ strain = \frac{V - V_o}{V_o}$$

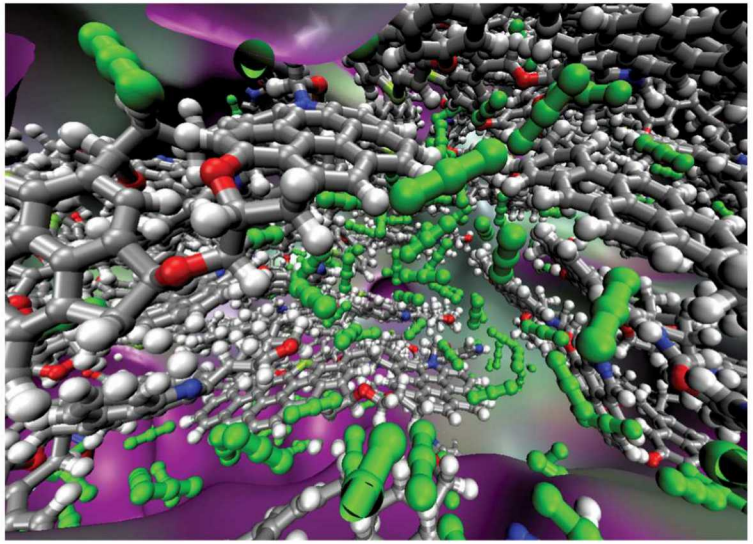
V: kerogen volume after gas adsorption

V_o: kerogen volume before gas adsorption

Chemo-mechanical coupling in kerogen gas adsorption (PCCP 20, 11390, 2018)







Highlighting shale gas research from the Geoscience Group, Sandia National Laboratories, NM, USA. This work was conducted by Dr Tuan Ho, thanks to funding granted to Dr Yifeng Wang by the DOE National Energy Technology Laboratory.

Chemo-mechanical coupling in kerogen gas adsorption/desorption

We use an integrated experimental and modeling approach to fundamentally understand the interaction of gas and fluid with kerogen and clay under reservoir conditions. Specifically, nanostructural properties of subsurface porous media, gas adsorption and release from the kerogen network, deformation of shale associated with adsorption and lithostatic stress, and wettability of inorganic and organic matter.

As featured in:

See Tuan Anh Ho *et al.*, *Phys. Chem. Chem. Phys.*, 2018, **20**, 12390.

ROYAL SOCIETY OF CHEMISTRY

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Upon shale gas extraction kerogen shrinks

Summary

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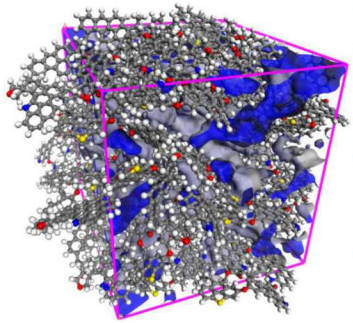
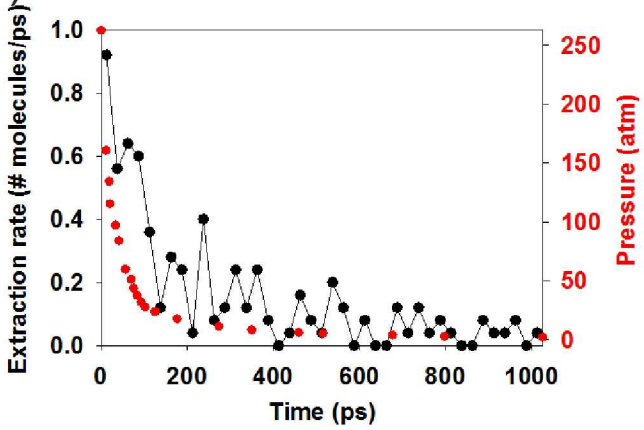
1. Nanostructure of kerogen

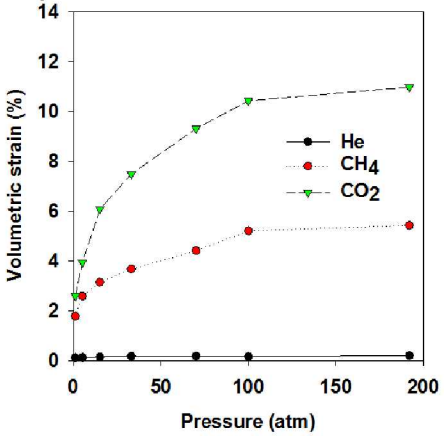
(Sci. Rep. 2016)





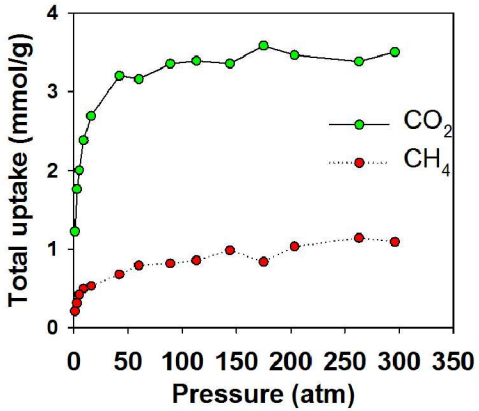
3. Kerogen swelling

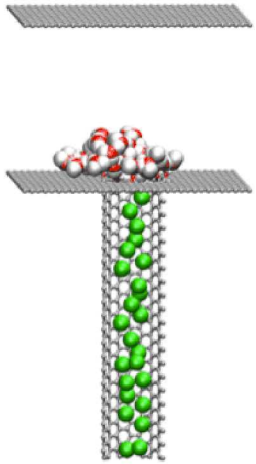
(PCCP 2018)

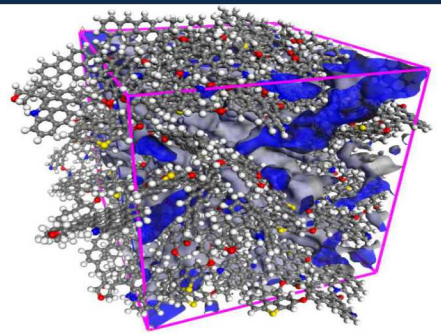


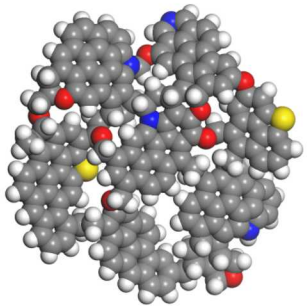
2. CH_4/CO_2 adsorption onto kerogen

(Fuel 2018)









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