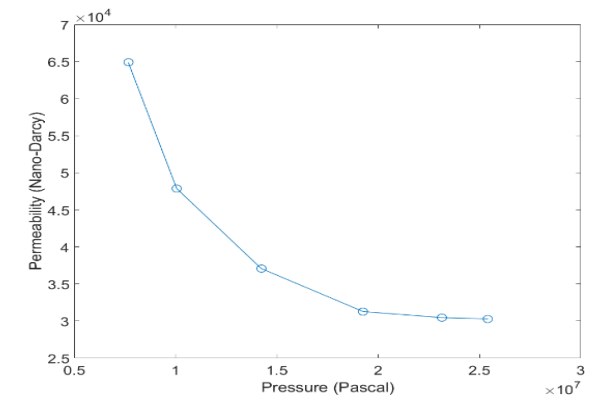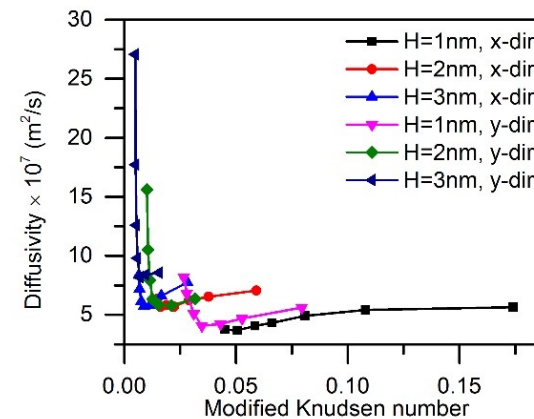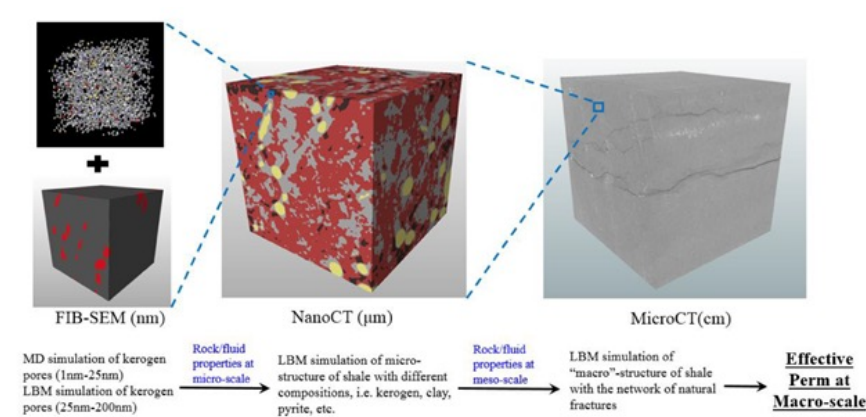# Dr. Guan Qin (Professor)

- Multi-scale and multi-physics numerical modeling of coupled reactive transport subsurface processes
  - Molecular simulation
  - Lattice Boltzmann (LB) methods and simulation
  - Finite element/finite difference methods
  - Upscaling processes
- One example – Permeability estimation for shales (SPE 181689)

FIB-SEM (nm)    NanoCT (μm)    MicroCT(cm)

MD simulation of kerogen pores (1nm-25nm)
LBM simulation of kerogen pores (25nm-200nm)

Rock/fluid properties at micro-scale

LBM simulation of micro-structure of shale with different compositions, i.e. kerogen, clay, pyrite, etc.

Rock/fluid properties at meso-scale

LBM simulation of "macro"-structure of shale with the network of natural fractures

Effective Perm at Macro-scale

Legend:
- H=1nm, x-dir
- H=2nm, x-dir
- H=3nm, x-dir
- H=1nm, y-dir
- H=2nm, y-dir
- H=3nm, y-dir

Diffusivity $\times 10^7$ (m$^2$/s) vs Modified Knudsen number

Permeability (Nano-Darcy) vs Pressure (Pascal)
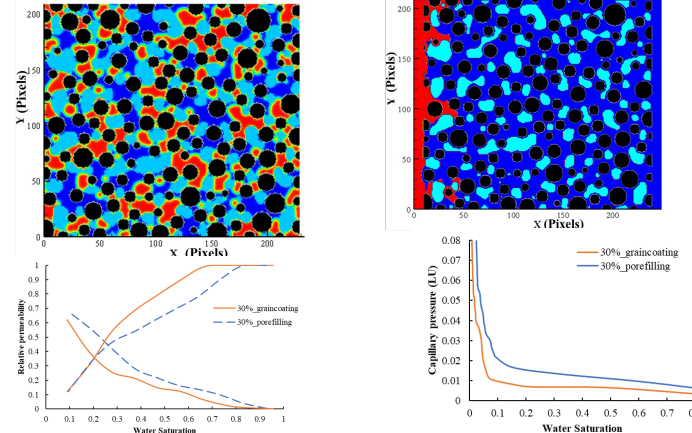
# Guan Qin's Research Applications

Molecular Simulation on Multi-functional Proppant for $CO_2$ Sequestration
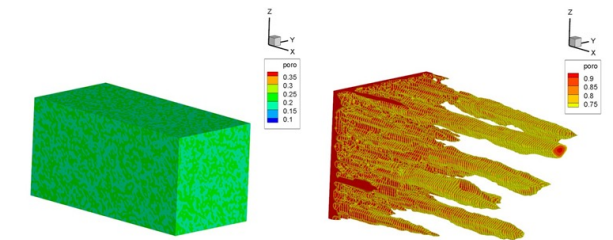**Fuel** Vol 249, 2019, Vol 292, 2021
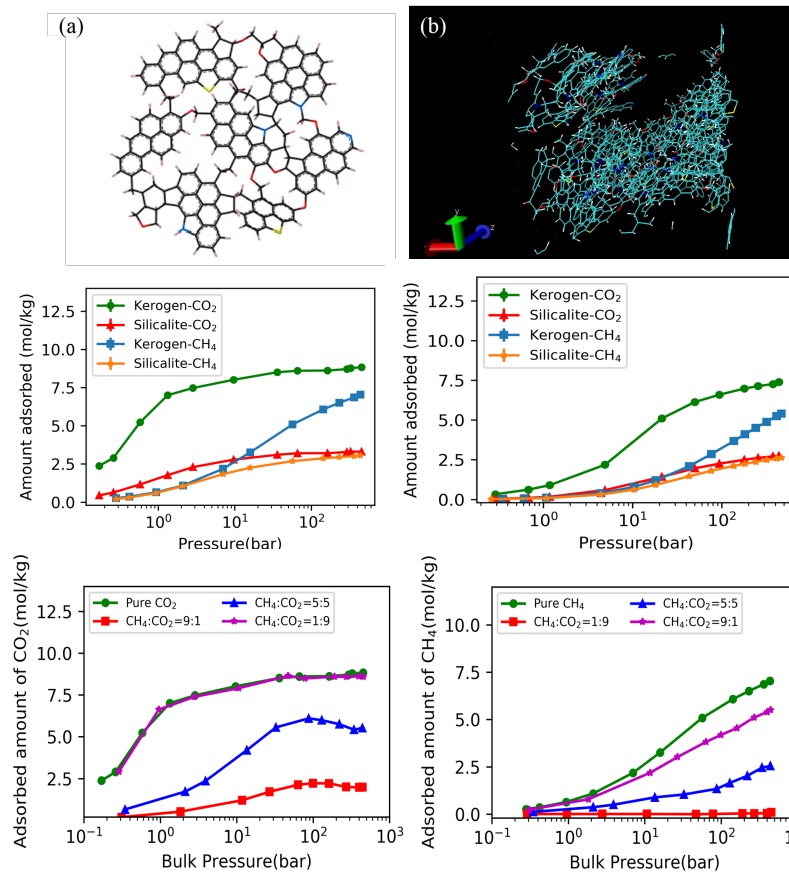


Molecular Simulation on $CO_2/CH_4$ Exchange in Hydrates
SPE 195457



(a) Beginning
(b) 100 ns
(c) 200 ns
(d) 250 ns
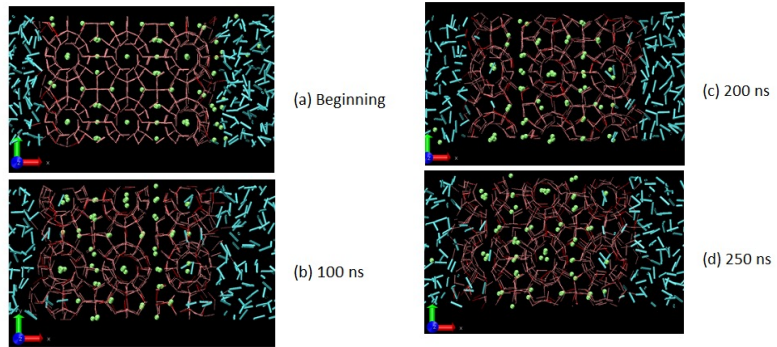
LB Simulation for Estimating Hydrate Permeability and Capillary Pressure
SPE 209395



Reactive Transport Modeling of Dissolution Processes in Carboante Formation
SPE 185845



Reactive Transport Modeling of Matrix Acidizing Stimulation
SPE 199262



(a)
(b)
(c)
(d)