

TXLA CMC Monthly Meeting

Texas A&M University - Kingsville

Jong-Won Choi

J. Louise Liu

February 13, 2024

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Texas A&M University – Kingsville

- Member of Texas A&M University System
- **Minority Serving Institution**
 - Total enrollment: 5681 (Spring 2023)
 - Hispanic: 3851 (69%);
 - African-American: 215 (4%)
- Undergraduate, graduate, and Ph.D. programs



■ Jong-Won Choi

- Associate professor in the Department of Civil and Architectural Engineering
- Worked on **SECARB project** at BEG: 2008 - 2012
- **Geomechanics**: stress field in response to pore pressure change in geologic formations
- **Micromechanics**: interaction between micro-heterogeneities (e.g., swelling clay particles) and its impact on stress field in a continuum

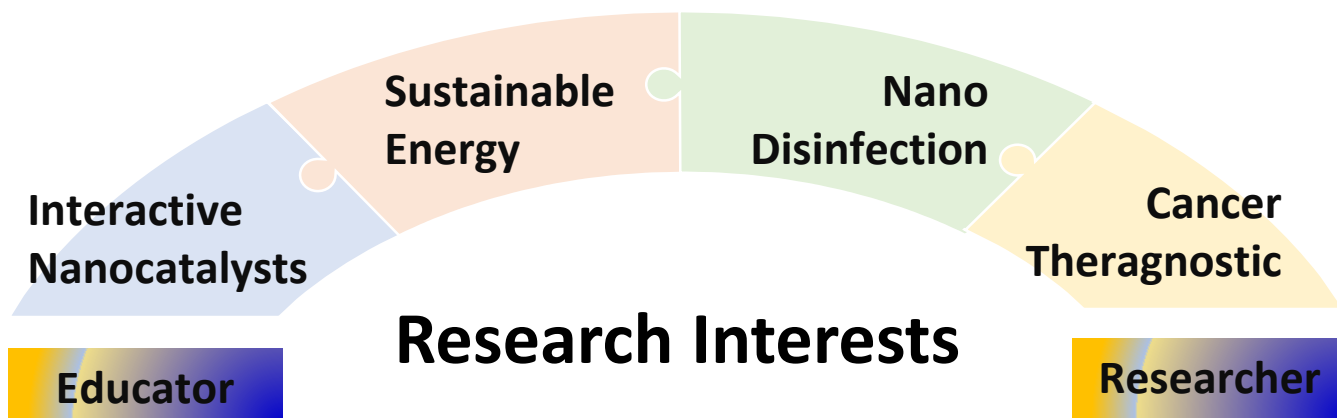
■ J. Louise Liu

- Professor in the Department of Chemistry and TAMU Energy Institute
- Worked on the porous materials for **carbon capture and sequestration** (e.g. Metal-organic Frameworks (MOFs), ACS PRFs)
- **Materials design:** bottom-up and top-down synthesis in conjunction with artificial intelligence and lab automation
- **Materials evaluation:** nano-structural characterization
 - Crystallographic characterization (X-ray powder and single crystal diffraction)
 - Porosity measurement (BET)
 - Spectroscopic analyses (FT-IR and NMR)
- Electrochemical performance of the catalysts and devices

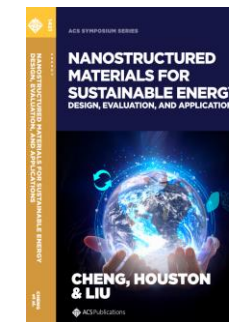
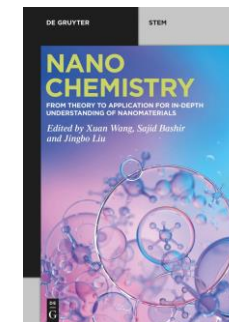
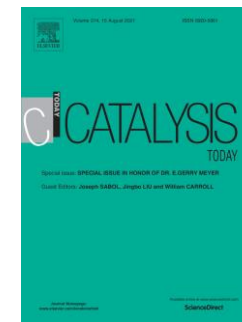
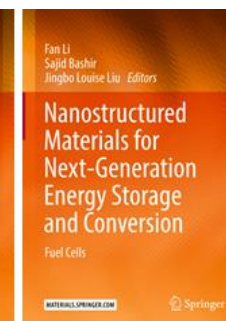
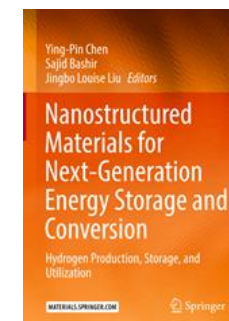
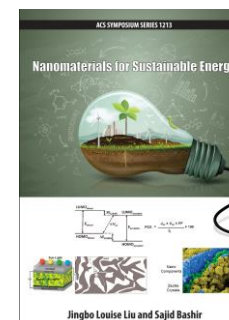
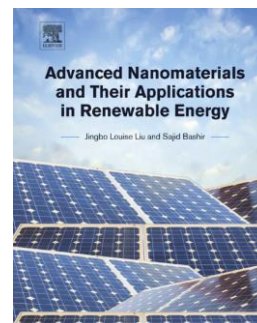
Jingbo Louise Liu: Education Background and Research Interests

Dr. J. Louise LiU (*Lithium-Uranium*), Full Professor

- ✓ 2023 Distinguished service award of Energy and Fuels, the American Chemical Society (ACS)
- ✓ 2023 E. Ann Nalley Southwest Regional Award to ACS for volunteer service
- ✓ 2023 Women of the Year, Texas Diversity Council
- ✓ Fellows of three societies: ACS, Linnean Society, & RSC;
- ✓ Chartered Scientist & Chartered Chemist;
- ✓ Faculty Fellowship Summer Institute in Israel;
- ✓ Fellow of Japan Society for the Promotion of Science;
- ✓ US ONR distinguished fellow and Air Force DEBI faculty fellow;
- ✓ Councilor of Energy and Fuels, & ACS career consultant; and
- ✓ 2021 Distinguished Women in Chemistry/Chemical Engineering, International Union of Pure and Applied Chemistry (IUPAC).



- 1) J. Liu, S. Bashir, and J. C Wigle, US 2019 / 0094241 A1, Ytterbium as a Surrogate Calcium Ion To Investigate Calcium Based Transduction.
- 2) J. Sabol, C. William, J. Liu (Managing Guest Editor), Gateway to Novel Energy Conversion Technology In Honor of Dr. E. G. (Gerry) Meyer, Special Issue, *Catalysis Today*, 2021.



Outreach Activities

- **Collaboration with a DAC project for training**
 - South Texas DAC Hub (in award negotiation)
 - Will provide students with **internship opportunities**
 - **Site visit** as a part of undergraduate/graduate courses

- **Community engagement**
 - Recruitment of students from **underrepresented minority groups and local communities**
 - Recruitment of students from the professional symposia
 - Presentation at the local high schools

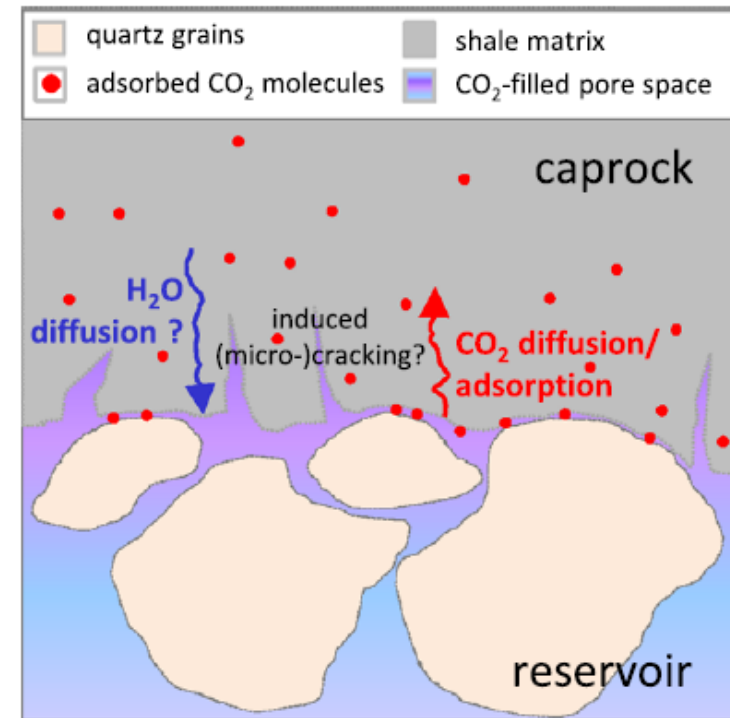
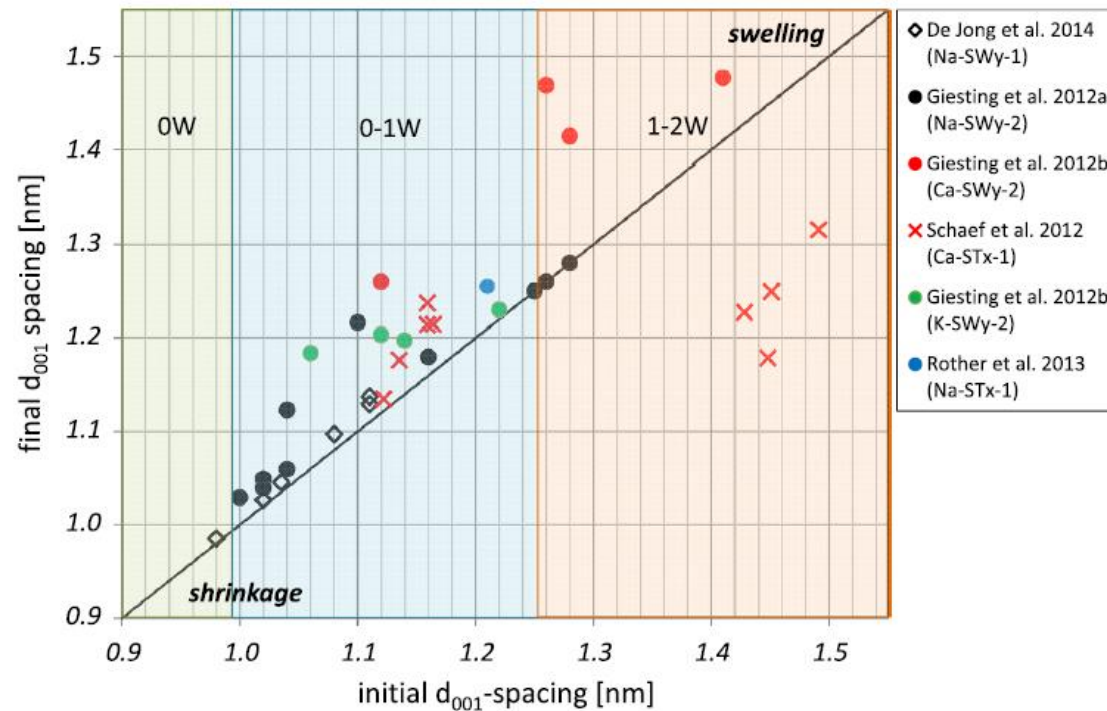
Outreach Activities (Liu)

- **Collaboration with a TAMU Chemistry and Energy Institute**
 - Hydrogenase-coordinated MOFs for carbon capture and conversion
 - MOFs synthesis and evaluation to improve carbon capture efficiency (Decarbonization)
 - Student summer fellowships and/or internship opportunities (DOE, DOD/DHS, ExxonMobil, Shell)
 - Collaboration with DOE lab scientists to provide training for undergraduate/graduate (through course work)
 - Collaboration with professional society to provide career consultation (Dr. Liu is one of the ACS career consultants)

Research Problem

■ Swelling of clay minerals

– Swelling due to sorption of CO₂ molecules



[Busch et al., 2016]

Research Plan (Liu)

■ Molecular Dynamics simulation

- Crystallographic investigation (octahedral and tetrahedral) of clay minerals, before and after CO₂ capture
 - Na-rich montmorillonite (Focus for Yr 1)
 - Mg/Ca-rich and Al-rich montmorillonite (Focus for Yr 2)
- Investigation of **interaction between CO₂ molecules and clay minerals**
- Key points of Molecular Dynamics Simulation
 - CO₂ Intercalation in hydrated Na-rich Montmorillonite (as a demonstration)
 - Methods: Classical Force Fields and Density Functional Theory (for comparison)
 - Short/long-range Interaction Algorithms
- Experimental verification of BET

Research Plan (Liu)

- Clay specimen (starting point)
 - Na-rich montmorillonite (Na-rich-MMT (SWy-2) from Wyoming)
 - Ca-rich montmorillonite (Ca-rich-MMT (STx-1b) from Texas)
- Variables of CO₂ exposure to clay minerals
 - The duration of exposure of the clay samples: 8-12 hours
 - The pressure of CO₂: 1500 psig (~10 Mpa, scCO₂)
 - The test temperature: 55 °C
- Anticipated results
 - Interlayer content & basal d-spacing (d-spacing of 001 plane: 10 Å without adsorption, adsorbed gases CO₂ or H₂O: 11.5-12.5 Å)
 - Changes in porosity, permeability, and formation of microfractures in cap rocks

Anticipated Results (Liu)

Space Group:
C2/m

Crystal System:

Monoclinic

a: 5.2000 Å

b: 9.2000 Å

c: 10.1300 Å

β : 99.00 °

Cell Volume:

478.653 Å³

Asymmetric Unit:

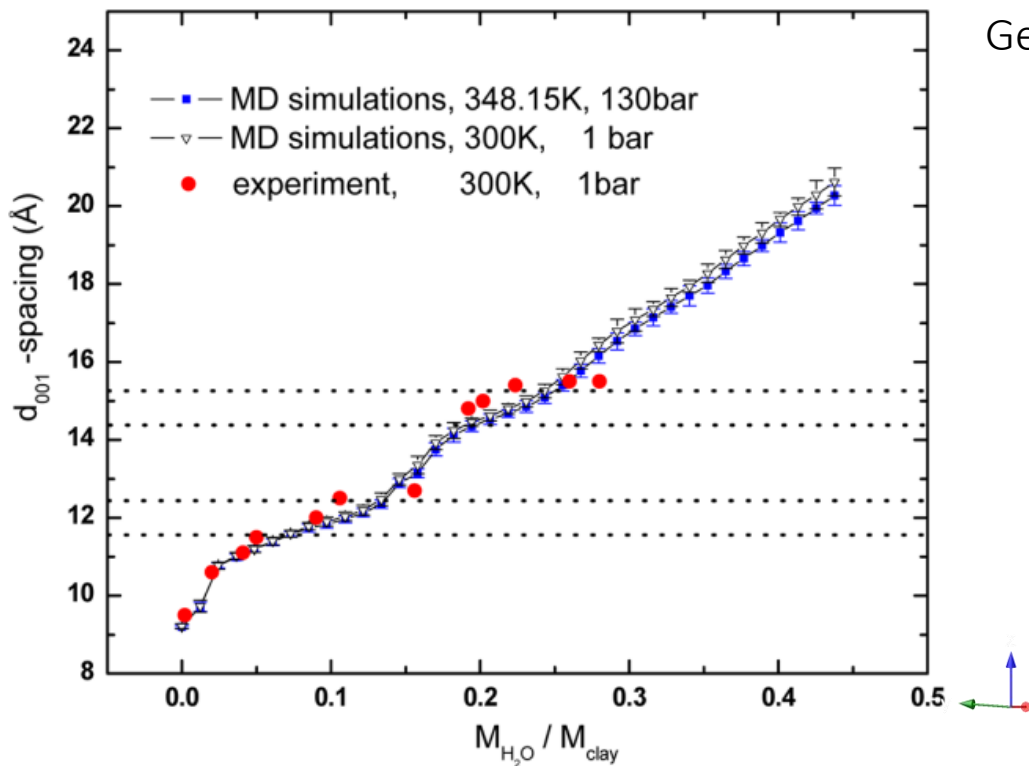
8 sites

Unit Cell: 40 sites

per unit cell

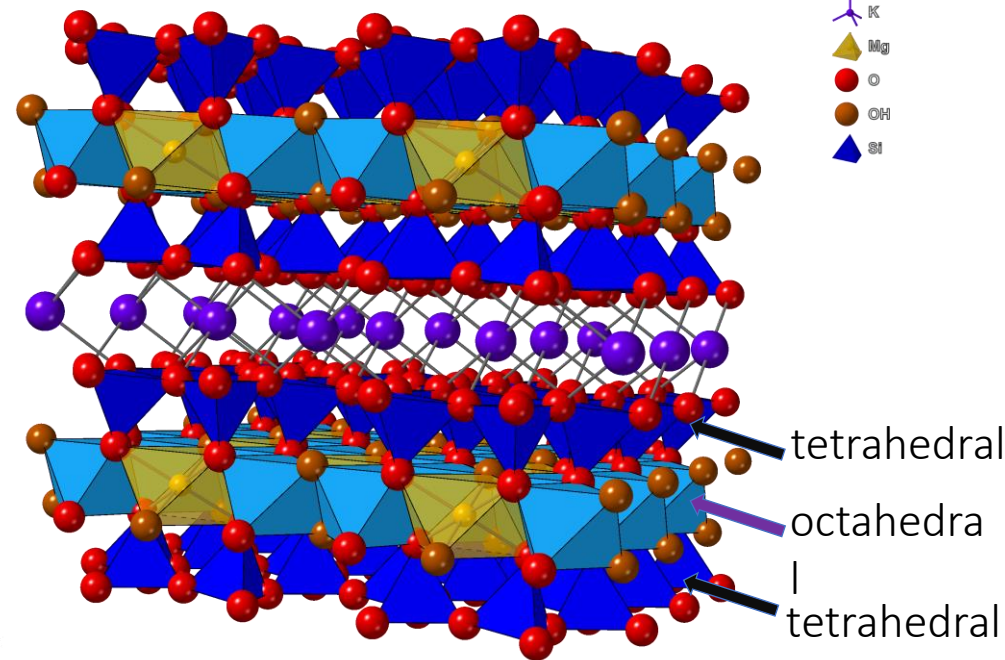
Density: 2.9402

g/cm³



Swelling behavior of Na-montmorillonite clay upon hydration

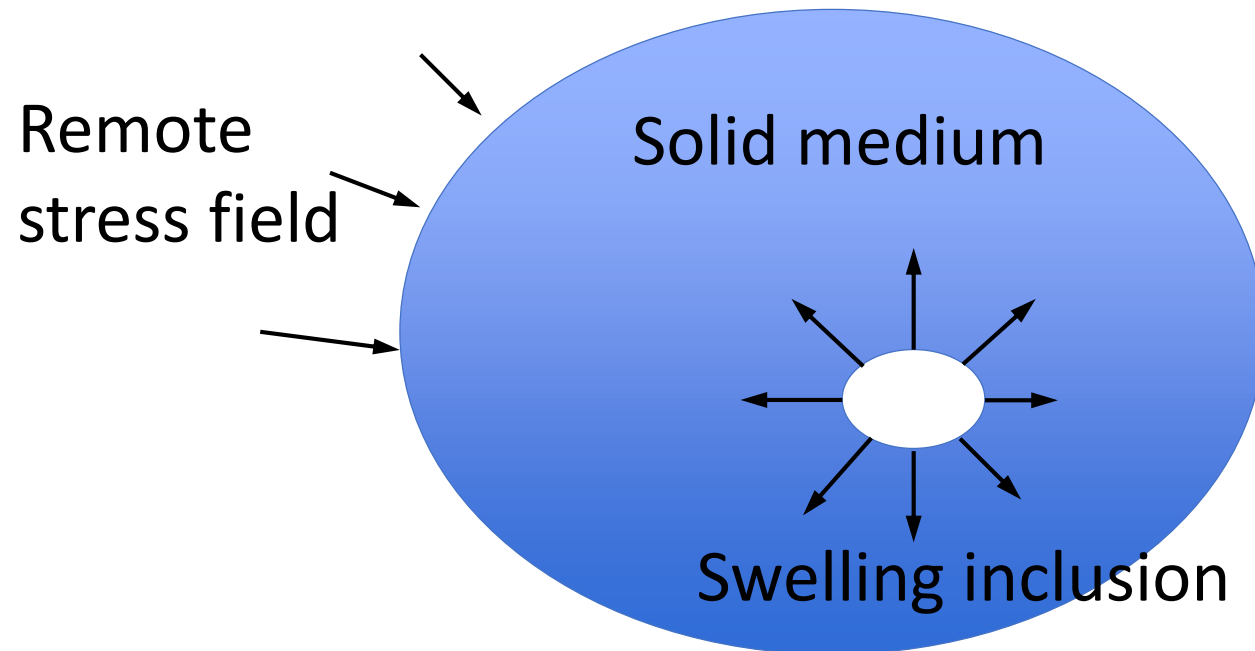
General formula: (Al,Mg)(Si,Al)O₁₀(OH)₂K_{0.58}



Crystalline structure of Montmorillonite

Research Plan (Choi)

- **Numerical integration of a Green's function in 3D space**
 - Anisotropic solid medium
 - Infinite domain with remote stress field
 - Calculate changes in stress-field around swelling cavities



$$G_{ij}(\vec{x}, \vec{y}) = \frac{1}{16\pi\mu(1-\nu)r} \left[(3-4\nu)\delta_{ij} + \frac{(x_j - y_j)(x_k - y_k)}{r^2} \right]$$

Questions?

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