# Xiaohan (Sally) Li, Ph.D.

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Personal Webpage | Google Scholar | ResearchGate

Education	
• Ph.D. in Civil and Environmental Engineering, Princeton Unive	rsity 2018-2023
- Advisor: Ian C. Bourg	
• B.S. in Energy and Resources Engineering, Peking University, C	Thina 2014-2018
- Research Advisor: Dongxiao Zhang; Wei Kang	
• B.S. in Economics, Peking University, China	2015-2018
Academic Appointment & Experience	
• CIMES Postdoc Research Associate, Princeton University/NOA	A GFDL 2023-present
- Host: Paul Ginoux	
• Visiting Scholar, Texas A&M University	2023
- Host: Yue Zhang	
Honors & Awards	
• C. Ellen Gonter Award, American Chemical Society	2023
• CEE Departmental Travel Award, Princeton University	2022
• SEAS Travel Grants, Princeton University	2022
• Walbridge Fund Graduate Award for Environmental Research	2021
• Merit Student, Peking University	2014-2018 (4 times)
• National Encouragement Scholarship, China	2014-2018 (4 times)
• Cyrus Tang Scholarship, China	2014-2018 (4 times)
• Meritorious Winner, International Mathematical Contest in Mod	deling, COMAP 2016

• 2nd Prize in National College Students Physics Competition, China

2015

## **Publications**

#### Published

- 1. **Li, X.**, Bourg I.C. Hygroscopic growth of adsorbed water films on smectite clay particles. *Environmental Science & Technology*, 58, 2, 1109–1118 (2024).
- 2. **Li**, **X**. Water, salt, organics, and minerals: improved understanding of aerosol microphysics from a nanoscale basis. *Princeton University* (2023).
- 3. Li, X., Bourg I.C. Phase State, surface tension, water activity, and accommodation coefficient of water-organic clusters near the critical size for atmospheric new particle formation. *Environmental Science & Technology*, 57, 13092-13103 (2023).
- 4. **Li, X.**, Bourg I.C. Microphysics of liquid water in sub-10 nm ultrafine aerosol particles. *Atmospheric Chemistry and Physics*, 23, 2525-2556 (2023).
- 5. Wu Y., Li P., Yan B., Li, X., Huang Y., Yuan J., Feng X., Dai C. A Salt-Induced Tackifying Polymer for Enhancing Oil Recovery in High-Salt Reservoirs: Synthesis, Evaluation, and Mechanism. *Green Energy & Environment*, in press (2023).
- Zhou S., Zhang D., Wang H., Li, X. A modified BET equation to investigate supercritical methane adsorption mechanisms in shale. *Marine and Petroleum Geology*, 105, 284-292 (2019).

2020

# Teaching/Mentoring Experience

## Teaching Assistant

• CEE207: "Intro to Environmental Engineering", Princeton University

#### Undergraduate Research Advising

- Yuno Iwasaki, Physics, Class of 2023
- George Dickinson, Civil and Environmental Engineering, Class 2023
- Benjamin Henry, Civil and Environmental Engineering, Class 2022

#### Service and Outreach

- Journal Reviewer: Journal of the American Chemical Society (JACS), ACS Omega
- Committee: AOS Diversity, Equity, and Inclusion (DEI) Committee, Princeton University.
- Organizer: Environmental Certificate Colloquium, High Meadow Environmental Institute, Princeton University. 2021-2022
- Co-Chair: AGU Fall Meeting, Session A35N: Molecular-Scale Characterization of Atmospheric Aerosol Using Simulations and Experiments.
- Organizer: EEWR Brown Bag Seminar, Civil and Environmental Engineering, Princeton University. 2020-2021

## Skills

#### Computational Skills

- Climate modeling
- MD simulations and DFT: LAMMPS, Gromacs, Quantum Espresso
- Computational fluid dynamics: OpenFOAM
- Machine learning and finite element analysis programming: Python, Matlab, C++/C

#### **Experimental Skills**

- Pore structure characterization of minerals: mercury intrusion porosimeters, advanced micropore size and chemisorption analyzer
- High pressure gas and sub-critical fluid sorption measurement: rubotherm gravimetric adsorption instruments

#### Presentations

- 1. **Li, X.**, Bourg I.C. Hygroscopic growth of adsorbed water films on smectite clay particles. ACS Spring Meeting, New Orleans, March, 2024 (Oral).
- 2. Li, X. Water, salt, and organics in nano-aerosol particles: improved understanding of aerosol microphysics from molecular basis. University of Washington in St. Louis, Missouri, April 2023 (Oral).
- 3. Li, X., Bourg I.C. How does water contribute to new particle formation? ACS Spring Meeting, Indianapolis, March 2023 (Oral).
- 4. **Li, X.** Aerosol microphysics from molecular understanding to improved representation in climate models. Geophysical Fluid Dynamics Laboratory, NOAA, Princeton, February 2023 (Oral).
- 5. **Li, X.**, Bourg I.C. Molecular dynamics simulations of the microphysics of liquid water in nano-aerosol droplets. AAAR 40th Annual Conference, Raleigh, October 2022 (Oral).
- 6. Li, X., Bourg I.C. Molecular dynamics simulations of the effect of surface charge density and oxidation degree on the colloidal stability of graphene oxide. Goldschmidt, Honolulu, July 2022 (Poster).
- 7. Li, X., Bourg I.C. Molecular dynamics simulations of water, salt, and organics in nano-aerosol particles. ACS Spring Meeting, San Diego, March 2022 (Oral).
- 8. Li, X., Bourg I.C. Molecular dynamics simulations of liquid water microphysics in nano-aerosol droplets. AGU Fall Meeting, New Orleans, December 2021 (Poster).
- 9. **Li, X.**, Bourg I.C. Molecular dynamics (MD) simulation of the microphysics of liquid water in aerosol particles. SMatCH Seminar, Princeton University, November 2021 (Oral).

- 10. Li, X., Bourg I.C. Phase-mixing states in secondary organic aerosol: key to water cloud condensation and optical insights. EEWR Brown Bag Seminar, Princeton University, December 2019 (Oral).
- 11. Li, X., Bourg I.C. How secondary organic aerosol affects precipitation and radiative forcing. AGU Fall Meeting, San Francisco, December 2019 (Poster).

# Research Experience

#### Sahel Drought and Climate Internal Variability

Advisor: Paul Ginoux, NOAA GFDL

2023/09-Present

• Characterizing the impact of multidecadal climatic variability on the dust emission activity and drought index in Sahel region using GFDL earth system model ESM4.1.

#### Aerosol Microphysics in Climate Models

Advisor: Paul Ginoux and Fabien Paulot, NOAA GFDL

2023/09-Present

• Implementing a two-moment aerosol microphysics scheme in GFDL climate model.

## Ice Nucleation of Organic Aerosols

Collaborator: Prof. Yue Zhang, Texas A&M University

2023/01-2023/08

• Developed parameterization of the ice nucleation ability of organic aerosols as a function of their phase state.

#### Water Films on Smectite Clay

Advisor: Prof. Ian Bourg, Princeton University

2022/09-2023/05

- Investigated water film disjoining pressure on smectite clay across varying salinities and counterions.
- Analyzed hygroscopic growth patterns of diverse dust particles.

#### **Atmospheric New Particle Formation**

Advisor: Prof. Ian Bourg, Princeton University

2022/03-2022/08

- Conducted MD simulations on water-organic clusters (1-4 nm) to study phase-mixing states and water uptake dynamics.
- Reconciled discrepancies between experimental measurements and MD simulations using modified classical theories.

#### Black Carbon Aggregation in Aerosol Droplets

Advisor: Prof. Ian Bourg, Princeton University

2021/10-2022/06

- Examined black carbon particle phase-mixing in aerosol droplets using MD simulations.
- Developed a morphology phase diagram for black carbon particles using the SVM method.

#### Microphysics of Liquid Water in Ultrafine Aerosol Particles

Advisor: Prof. Ian Bourg, Princeton University

2018/09-2021/10

- Investigated thermodynamic and kinetic properties of sub-10 nm droplets with varying NaCl concentrations and sizes.
- Explored deviations of Kelvin and Köhler theory predictions at nanoscale due to salinity and organic coatings.

#### Methane Adsorption Mechanisms in Shale

Advisor: Prof. Dongxiao Zhang, Peking University

2017/03-2018/06

- Proposed a modified BET equation for high-pressure multi-layer methane adsorption.
- Characterized shale storage capacity for CH<sub>4</sub> through high-pressure adsorption experiments.

# Water Sensitivity and Mechanical Properties of Sedimentary Rocks

Advisor: Prof. Dongxiao Zhang, Peking University

2016/12-2017/06

- Developed an anisotropy-inclusive multi-scale effective stress formulation.
- Conducted microcantilever beam loading tests under ESEM conditions.

#### Pore Structure Characterization of Sedimentary Rocks

Advisor: Prof. Dongxiao Zhang, Peking University

2015/05-2017/10

- Introduced a complex-pore-characterization model for shale to mitigate tension strength effects.
- Performed mercury intrusion and low-pressure N2 and CO2-adsorption experiments on terrestrial and oil shale samples.