

Xiaohan (Sally) Li, Ph.D.

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Education

- Ph.D. in Civil and Environmental Engineering, Princeton University 2018-2023
– **Advisor:** Ian C. Bourg
- B.S. in Energy and Resources Engineering, Peking University, China 2014-2018
– **Research Advisor:** Dongxiao Zhang
- B.S. in Economics, Peking University, China 2015-2018

Academic Appointment & Experience

- CIMES Postdoc Research Associate, Princeton University/NOAA GFDL 2023-present
– **Supervisor:** Paul Ginoux
- Visiting Scholar, Texas A&M University 2023
– **Host:** Yue Zhang

Honors & Awards

- CEE Departmental Travel Award, Princeton University 2022
- SEAS Travel Grants, Princeton University 2022
- Walbridge Fund Graduate Award for Environmental Research, Princeton University 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 Modeling, COMAP 2016
- Outstanding Counselor, Peking University 2015
- 2nd Prize in National College Students Physics Competition, China 2015

Publications

Published

1. 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).
2. **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).
3. **Li, X.**, Bourg I.C. Microphysics of liquid water in sub-10 nm ultrafine aerosol particles. *Atmospheric Chemistry and Physics*, 23, 2525-2556 (2023).
4. 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).

In Review

1. **Li, X.**, Bourg I.C. Hygroscopic growth of adsorbed water films on smectite clay particles. *Environmental Science & Technology*, in review (2023).

In Preparation

1. **Li, X.**, Bourg I.C. Molecular insights into the black carbon aggregation process and phase-mixing state in aerosol droplets. *Journal of Physical Chemistry A*, in preparation.
2. **Li, X.**, Steinke I., Zhao J., Roesch C., Zhang Z., Surratt J., Cziczo D., Burrows S., Zhang Y. Quantifying the Effects of Phase State on the Deposition Ice Nucleation Abilities of Organic Aerosols. *Environmental Science & Technology*, in preparation.
3. **Li, X.**, Zhang S., Li P., Jiang Z., Zhang D. Reassessing CO₂ storage capacity based on a modified physisorption model for surface area and porosity determination. *Environmental Science & Technology*, in preparation.
4. Liu Y., **Li, X.**, Zhang S. Dimensionless parametrization of ice nucleation in mixed-phase clouds. *Atmospheric Chemistry and Physics*, in preparation.

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

Talks / Presentations

1. **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 (**invited**).
2. **Li, X.**, Bourg I.C. How does water contribute to new particle formation? ACS Spring Meeting, Indianapolis, March 2023.
3. **Li, X.** Aerosol microphysics from molecular understanding to improved representation in climate models. Geophysical Fluid Dynamics Laboratory, NOAA, Princeton, February 2023 (**invited**).
4. **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.
5. **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.
6. **Li, X.**, Bourg I.C. Molecular dynamics simulations of water, salt, and organics in nano-aerosol particles. ACS Spring Meeting, San Diego, March 2022.
7. **Li, X.**, Bourg I.C. Molecular dynamics simulations of liquid water microphysics in nano-aerosol droplets. AGU Fall Meeting, New Orleans, December 2021.
8. **Li, X.**, Bourg I.C. How Secondary Organic Aerosol Affects Precipitation and Radiative Forcing. AGU Fall Meeting, San Francisco, December 2019.

Teaching Experience

Teaching Assistant

“Intro to Environmental Engineering,” Instructor: Prof. Ian Bourg, Princeton University 2020

Undergraduate Research Advising

G Dickinson, B Henry, Y Iwasaki. Summer research internships, HMEI 2020

Service and Outreach

- **Organizer:** EEWR Brown Bag Seminar, Civil and Environmental Engineering, Princeton University. 2020-2021
- **Co-Chair:** AGU Fall Meeting, Session A35N: Molecular-Scale Characterization of Atmospheric Aerosol Using Simulations and Experiments. 2021
- **Organizer:** Environmental Certificate Colloquium, High Meadow Environmental Institute, Princeton University. 2021-2022
- **Journal Reviewer:** ACS Omega

Research Experience

Sahel Drought and Climate Internal Variability

Co-authors: Paul Ginoux, John Dunne, 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

Co-authors: Paul Ginoux, 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 CH₄ through high-pressure adsorption experiments.

Water Sensitivity and Mechanical Properties of Shale

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 Shale

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.