

Xiaohan (Sally) Li

Ph.D.

Atmospheric and Oceanic Program

Princeton University

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EDUCATION

- Ph.D. in Civil and Environmental Engineering, Princeton University (2018-2023)
- B.S. in Energy and Resources Engineering, Peking University, China (2014-2018)
- B.S. in Economics, Peking University, China (2015-2018)

ACADEMIC APPOINTMENT

- CIMES Postdoc Research Associate, Princeton University/GFDL (2023-2024)

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
- National Encouragement Scholarship, China, 2014-2018
- Cyrus Tang Scholarship, China, 2014-2018
- 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

1. **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 (35), 13092-13103 (2023).
2. **Li X.**, Bourg I.C. Microphysics of liquid water in sub-10 nm ultrafine aerosol particles. *Atmospheric Chemistry and Physics*, 23, 2525-2556 (2023).
3. 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).

PUBLICATIONS IN REVIEW

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 review, [preprint](#) (2023).

PUBLICATIONS IN PREPARATION

1. **Li X.**, Bourg I.C. Hygroscopic growth of adsorbed water films on smectite clay particles. *Environmental Science & Technology*, in preparation (2023).
2. **Li X.**, Zhang Y., Shrivastava M., Wolf M., Steinke I., Zhang Z., Surratt J., Cziczo D., Burrows S. Quantifying the Effects of Phase State on the Deposition Ice Nucleation Abilities of Organic Aerosols. *Environmental Science & Technology*, in preparation (2023).
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 (2023).

SKILLS

Computational skills

- 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

INVITED 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.
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.
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.

RESEARCH EXPERIENCE

Impact of ions on the energetics of water films on smectite clay

Advisor: Prof. Ian Bourg, Princeton University

2022/09-2023/5

- Examined the disjoining pressure of water films adsorbed on smectite clay as a function of salinity (0 to 1 M) and counterion type (Na, K, Ca).
- Characterized the hygroscopic growth of different dust particles type as a function of relative humidity.

How does water contribute to atmospheric new particle formation?

Advisor: Prof. Ian Bourg, Princeton University

2022/03-2022/08

- Performed MD simulations of water-organic clusters in the range of 1 to 4 nm to investigate the influence of water content on the phase-mixing states and water uptake thermodynamic and kinetics of the clusters.
- Examined the extent to which the properties of nano-clusters can be modeled by simple modifications of classical mean-field theories, and reconciled the discrepancies between previous experimental measurements and MD simulation studies.

Molecular insights into the black carbon aggregation process and phase-mixing state in aerosol droplets

Advisor: Prof. Ian Bourg, Princeton University

2021/10-2022/06

- Performed MD simulations to examine the impact of water content, and the O/C ratio and charge density of black carbon particles on the phase-mixing state of aerosol droplets.
- Constructed the morphology phase diagram of black carbon particles as a function of O/C ratio, charge density and droplet size by supportive vector machine (SVM) method.

Microphysics of liquid water in sub-10 nm ultrafine aerosol particles

Advisor: Prof. Ian Bourg, Princeton University

2018/09-2021/10

- Performed MD simulations of sub-10 nm droplets with different NaCl concentration, different organic content and different size, and investigated the thermodynamic and kinetic property differences of nanoparticles with macroscopic bulk solutions.

- Investigated how salinity and organic coating deflect Kelvin and Köhler theory prediction at nanometer scale.

A modified BET model to investigate supercritical methane adsorption mechanisms in shale

Advisor: Prof. Dongxiao Zhang, Peking University

2017/03-2018/06

- Proposed a modified BET equation describing high-pressure multi-layer methane adsorption.
- Conducted high-pressure adsorption experiments to characterize shale's storage capacity for CH₄.

Water sensitivity of terrestrial shale and its effect on multi-scale mechanical properties

Advisor: Prof. Dongxiao Zhang, Peking University

2016/12-2017/06

- Reformulated the multi-scale effective stress while taking anisotropy into consideration.
- Performed five pre-tests to load the microcantilever beams under ESEM.

Comprehensive study and characterization of the pore structure of terrestrial shale and marine shale

Advisor: Prof. Dongxiao Zhang, Peking University

2015/05-2017/10

- Developed a complex-pore-characterization model of shale to minimize tension strength effect.
- Conducted mercury intrusion experiments and low pressure N₂ and CO₂-adsorption experiments to characterize pore structures of 23 terrestrial shale samples and 9 oil shale samples.

INTERNSHIP/TEACHING EXPERIENCE

Data Scientist

Correlation One, New York (2022)

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)

ORGANIZING EXPERIENCE

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