KAIHANG SHI

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EDUCATION

Ph.D. North Carolina State University (NCSU), Raleigh, NC, USA — 2020
in Chemical and Biomolecular Engineering, GPA 4.0/4.0
Advisors: Prof. Keith E. Gubbins and Prof. Erik E. Santiso (co-advisor)

B.S. East China University of Science & Technology (ECUST), Shanghai, China — 2015
in Polymer Materials and Engineering
Advisors: Prof. Shuangliang Zhao and Prof. Honglai Liu

RESEARCH EXPERIENCE

Postdoctoral Scholar, Northwestern University, Evanston, IL, USA — Aug. 2020 – present
in Chemical and Biological Engineering with Randall Snurr

- Developed energy-based features for machine learning to predict adsorption and separation of complex molecules in diverse nanoporous materials.
- Applied molecular dynamics and mathematical models to understand molecular diffusion in porous materials.
- Co-led the development and management of a first-of-its-kind, online adsorption database "MOFX-DB".

Graduate Research Assistant, NCSU, Raleigh, NC, USA — Aug. 2015 – July 2020
in Chemical and Biomolecular Engineering with Keith Gubbins & Erik Santiso

- Developed novel theories and simulation techniques for adsorption on heterogeneous surfaces.
- Pioneered theoretical development of the unique microscopic pressure/stress tensor and its calculation in complex systems where long-range Coulombic interactions are present.
- Developed '2D-route' to the effective tangential pressure in thin films, using an accurate 2D equation of state.

Undergraduate Research Assistant, ECUST, Shanghai, China — Aug. 2013 – Aug. 2015
in State Key Laboratory of Chemical Engineering with Honglai Liu & Shuangliang Zhao

- Applied coarse-grained molecular simulations to investigate the industrial extraction process for caprolactam, adsorption dynamics of triblock copolymers, and the formation of polycation/DNA-like complex.

HONORS AND AWARDS

Academic Awards:

2021 **DOE Team Science Contest Winner (Team Leader)**, US Department of Energy (DOE).
One of 9 winners from 64 participating DOE centers and hubs.

2020 **James K. Ferrell Outstanding Ph.D. Graduate Award**, NCSU.
Awarded annually to the top Ph.D. graduate in the Department of Chemical and Biomolecular Engineering. I was invited to speak at the 2021 Spring Commencement Ceremony (video).

2019 **AIChE CoMSEF Graduate Student Award**, American Institute of Chemical Engineers (AIChE).
National recognition of excellence in graduate research, presented by The Computational Molecular Science and Engineering Forum (CoMSEF) at the AIChE annual meeting.

2018 **FOMMS Poster Prize**, Foundations of Molecular Modeling and Simulation (FOMMS) Meeting, Delavan, WI, USA.

2018 **Outstanding Poster Presentation Prize**, 8th International Workshop on Characterization of Porous Materials (CPM8), Delray Beach, FL, USA.

2014 **Cheng Siwei Chancellor's Fellowship**, ECUST.
The most prestigious annual award at ECUST.

2014 **Honorable Mention**, Mathematical Contest in Modeling, USA.
2014 **Special Prize for Academic Excellence (Top 1%)**, ECUST.

Teaching Awards:

2016 – 2018 **Mentored Teaching Fellowships (×3)**, NCSU.
Awarded to ten outstanding graduate students in the College of Engineering per semester to support extended teaching activities and course development.
2016 Fall **Linde Exceptional Teaching Assistant Award**, NCSU.
Only one recipient department-wide per semester.

Travel Grants:

2022 **FOA14 Travel Award**, 14th International Conference on Fundamentals of Adsorption, USA.
2019 Spring **Graduate Student Association Travel Assistance Award**, NCSU.
2018 **NSF Travel Award**, CPM8, USA.

PUBLICATIONS

9 × 1st author | 2 × co-1st author | 6 × 2nd author | 4 × corresponding author | Google Scholar
Double dagger (‡) denotes equal contribution; asterisk (*) denotes corresponding authors.

Book Chapter

1. **K. Shi***, E.E. Santiso, K.E. Gubbins, "Current Advances in Characterization of Nano-porous Materials: Pore Size Distribution and Surface Area", Chapter 12 in *Porous Materials: Theory and Its Application for Environmental Remediation*, Springer (2021): 315-340.

Peer-Reviewed Journal Publications

In preparation (manuscript available upon request):

20. R. Wang‡, **K. Shi**‡, J. Liu, R.Q. Snurr*, and J.T. Hupp*, "Atomic and Molecular Understanding of Vapor-Phase Nerve Agent Simulant Transport in Zr-MOF under Different Relative Humidity".
19. P. Seidel‡, **K. Shi**‡, C. Chmelik*, M. Goepel, R. Gläser, R.Q. Snurr, J. Kärger, "Diffusion and Adsorption of 2-Methylpentane and 3-Methylpentane in MFI-type Zeolite Crystals".

Published:

18. N.S. Bobbitt, **K. Shi**, B.J. Bucior, H. Chen, N. Tracy-Amoroso, Z. Li, Y. Sun, J.H. Merlin, J.I. Siepmann, D.W. Siderius, R.Q. Snurr*, "MOFX-DB: An Accessible Online Database of Computational Adsorption Data for Nanoporous Materials", *Journal of Chemical & Engineering Data,* 68 (2023): 483–498.
17. **K. Shi***, E.R. Smith*, E.E. Santiso, and K.E. Gubbins*, "A Perspective on Microscopic Pressure (Stress) Tensor: History, Current Understanding, and Future Challenges", *Journal of Chemical Physics*, 158 (2023): 040901 (**Invited Perspective, Editor's Pick, Featured on the journal cover**).
16. **K. Shi**, Z. Li, D.M. Anstine, D. Tang, C.M. Colina, D.S. Sholl, J.I. Siepmann, and R.Q. Snurr*, "Two-dimensional Energy Histograms as Features for Machine Learning to Predict Adsorption in Diverse Nanoporous Materials", *Journal of Chemical Theory and Computation*, in press (2023).
15. **K. Shi***, E.E. Santiso*, K.E. Gubbins*, "Can We Define a Unique Microscopic Pressure in Inhomogeneous Fluids?", *Journal of Chemical Physics*, 154 (2021): 084502.
14. P. Montero de Hijes, **K. Shi**, E.G. Noya, E.E. Santiso, K.E. Gubbins, E. Sanz, C. Vega*, "The Young-Laplace Equation for a Solid-Liquid Interface", *Journal of Chemical Physics*, 153 (2020): 191102.
13. **K. Shi***, Y. Shen, E.E. Santiso*, K.E. Gubbins*, "Microscopic Pressure Tensor in Cylindrical Geometry: Pressure of Water in a Carbon Nanotube", *Journal of Chemical Theory and Computation*, 16 (2020): 5548-5561.
12. S. Wang, **K. Shi**, A. Tripathi, U. Chakraborty, G.N. Parsons*, S.A. Khan*, "Designing PIM-1 Microfibers with Tunable Morphology and Porosity via Controlling Solvent/Nonsolvent/Polymer Interactions", *ACS Applied Polymer Materials*, 2 (2020): 2434-2443.
11. Y. Long, J.C. Palmer*, B. Coasne*, **K. Shi**, M. Sliwinska-Bartkowiak, K.E. Gubbins*, "Reply to the 'Comment on "Pressure Enhancement in Carbon Nanopores: A Major Confinement Effect"' by D. van Dijk, Phys. Chem.

Chem. Phys., 2020, 22, DOI: 10.1039/C9CP02890K", *Physical Chemistry Chemical Physics*, 22 (2020): 9826-9830.

10. J.D. Schneible, **K. Shi**, A.T. Young, S. Ramesh, N. He, C.E. Dowdey, J.M. Dubnansky, R.L. Lilova, W. Gao, E.E. Santiso, M. Daniele*, S. Menegatti*, "Modified Graphene Oxide (GO) Particles in Peptide Hydrogels: A Hybrid System Enabling Scheduled Delivery of Synergistic Combinations of Chemotherapeutics", *Journal of Materials Chemistry B*, 8 (2020): 3852-3868.
9. **K. Shi**, E.E. Santiso*, K.E. Gubbins*, "Conformal Sites Theory for Adsorbed Films on Energetically Heterogeneous Surfaces", *Langmuir*, 36 (2020): 1822-1838.
8. Z. Dai, D.T. Lee, **K. Shi**, S. Wang, H.F. Barton, J. Zhu, J. Yan, Q. Ke*, G.N. Parsons*, "Fabrication of Freestanding Metal-Organic Framework Predominant Hollow Fiber Mat and Its Potential Applications in Gas Separation and Catalysis", *Journal of Materials Chemistry A,* 8 (2020): 3803-3813.
7. C. Cutright, Z. Brotherton, L. Alexander, J. Harris, **K. Shi**, S. Khan, J. Genzer, S. Menegatti*, "Packing Density, Homogeneity, and Regularity: Quantitative Correlations between Topology and Thermoresponsive Morphology of PNIPAM-co-PAA Microgel Coatings", *Applied Surface Science*, 508 (2020): 145129.
6. **K. Shi**, E.E. Santiso*, K.E. Gubbins*, "Bottom-Up Approach to the Coarse-Grained Surface Model: Effective Solid–Fluid Potentials for Adsorption on Heterogeneous Surfaces", *Langmuir*, 35 (2019): 5975-5986.
5. K.E. Gubbins*, K. Gu, L. Huang*, Y. Long, J.M. Mansell, E.E. Santiso*, **K. Shi**, M. Śliwińska-Bartkowiak, D. Srivastava, "Surface-Driven High-Pressure Processing", *Engineering*. 4 (2018): 311-320. (Special issue on Green Industrial Processes).
4. **K. Shi**, K. Gu, Y. Shen, D. Srivastava, E.E. Santiso*, K.E. Gubbins*, "High-Density Equation of State for a Two-Dimensional Lennard-Jones Solid", *Journal of Chemical Physics*, 148 (2018): 174505.
3. Y. Xu, **K. Shi**, S. Zhao*, X. Guo, J. Wang*, "Block Length Determines the Adsorption Dynamics Mode of Triblock Copolymers to a Hydrophobic Surface", *Chemical Engineering Science*, 142 (2016): 180-189.
2. B. Zhan, **K. Shi**, Z. Dong, W. Lv, S. Zhao*, X. Han*, H. Wang, H. Liu, "Coarse-Grained Simulation of Polycation/DNA-Like Complexes: Role of Neutral Block", *Molecular Pharmaceutics*, 12 (2015): 2834-2844.
1. **K. Shi**, C. Lian, Z. Bai, S. Zhao*, H. Liu, "Dissipative Particle Dynamics Study of the Water/benzene/caprolactam System in the Absence or Presence of Non-ionic Surfactants", *Chemical Engineering Science*, 122 (2015): 185-196.

TEACHING EXPERIENCE

Invited Lecturer, 12/24-623 Molecular Simulation of Materials, Carnegie Mellon University 2020 Fall

- Presented **1** invited 110-minute lecture on microscopic pressure tensor.

Guest Lecturer, CHE315 Undergraduate Thermo I, NCSU 2020 Spring

- Presented **3** independent 50-minute lectures on classical thermodynamics.

Guest Lecturer, CHE713 Graduate Thermodynamics, NCSU 2016 – 2019 Fall

- Presented **18** independent 75-minute lectures on classical thermodynamics and statistical mechanics to more than 200 graduate students, most of whom are first-year Ph.D. students.

Guest Lecturer, CHE775 Multi-Scale Modeling of Matter, NCSU 2019 Spring

- Presented **1** independent 75-minute lecture on dissipative particle dynamics.

Teaching Assistant, CHE713 Graduate Thermodynamics, NCSU 2016 – 2018 Fall

- Delivered a one-hour hands-on tutorial on the high-pressure phase diagram each semester and developed interactive 3D models to help students understand the concept. I also led a 30-min "Problem Session" once a week on problem solving and collaborated on lectures, exams, and homework development.
- Select students' comments: 1). *Kaihang saved the course!* 2). *Kaihang is very passionate about Thermo and patiently explains complex material in a way that others can understand…I wish that he was the TA in every class that I have!*

Teaching Assistant, CHE331 Chemical Engineering Lab II, NCSU 2016 Spring

TRAINING IN PROPOSAL WRITING

Northwestern University, under the mentorship of Randall Snurr

- "Coordination-Chemistry-Derived Materials Featuring Nanoscale Porosity and Selective Chemical Separation Capabilities", *Department of Energy*, PIs: J. Hupp, R. Snurr and O. Farha (Awarded, 2022, DE-FG02-08ER15967). Contributions (~30%): Wrote two sections of the proposed research on xylene separation.
- "Modeling Metal-Organic Frameworks for Gas Storage, Separations, and Catalysis", *National Energy Research Scientific Computing Center*, PI: R. Snurr (Awarded 38,230 CPU node hours, 2021, ERCAP0020094). Contributions (~20%): Wrote an independent machine learning project on physics-inspired feature engineering.

North Carolina State University, under the mentorship of Keith Gubbins

- "Systems of Reduced Dimensionality: Thermodynamics, Transport and Potential for Nano-Scale Separations", *National Science Foundation*, PI: K. Gubbins (Unfunded, 2019).
  Contributions: Prepared figures and helped with polishing the proposal.
- "EAGER: Optimizing the Design of Reactive Adsorption Processes in Carbon Nanopores", *National Science Foundation*, PIs: K. Gubbins and E. Santiso (Unfunded, 2018).
  Contributions: Prepared figures and assisted with assembling the proposal.

MENTORING EXPERIENCE

Northwestern University

Mentored **2** undergraduate students: Priyen Shah (Summer 2022-), Julia Merlin (CoMSEF Scholars REU Program, Summer 2021, undergraduate student from Georgia Tech).

- Culminated with one peer-reviewed publication (DOI: 10.1021/acs.jced.2c00583).

North Carolina State University

Mentored **4** undergraduate students: Zongwei Huang (Summer 2018-2019, now Ph.D. student at the University of Michigan in Ann Arbor), Shicheng Li (Summer 2018), Kai Gu (Summer 2017, now Ph.D. student at University of Toronto), Yifan Shen (Summer 2017, now Ph.D. student at Johns Hopkins University).

- Culminated with two peer-reviewed publications (DOI: 10.1063/1.5029488, 10.1021/acs.jctc.0c00607) and another one paper in preparation.
- Encouraged students to pursue their career goals and facilitated their applications to graduate school.

LEADERSHIP, SERVICE, AND OUTREACH

DOE Basic Energy Sciences (BES) Early Career Network (ECN) Representative Oct. 2021 – Nov. 2022

- Served as the liaison between the Nanoporous Materials Genome Center (NMGC) and the DOE BES ECN.
- Led the organization of an invited webinar on grant writing for early career scientists, with a record number (~2,000) of attendees over Zoom (video).

Proposal Reviewer

- DOE Office of Science Graduate Student Research (SCGSR) program, 2021 Solicitation 2.

Journal Referee

- Reviewed >40 manuscripts for a total of 20 professional journals, including *Advanced Science*, *npj Computational Materials*, *Journal of Chemical Physics*, *Journal of Physical Chemistry Letters*, *Chemical Science*, *Journal of Colloid and Interface Science*, *Inorganic Chemistry Frontiers*, *New Journal of Physics*, *Journal of Computational Physics*.

Conference

- Chaired two invited sessions in honor of Keith Gubbins' 85th birthday at AIChE Annual Meeting, Phoenix, AZ, USA, 2022.
- Served as the poster judge at 14th International Conference on Fundamentals of Adsorption, USA, 2022.
- Co-chaired sessions "Applications of Molecular Modeling to Study Interfacial Phenomena" and "Molecular Simulation and Modeling of Complex Molecules" at AIChE Annual Meeting, Boston, MA, USA, 2021.

Volunteer with Habitat for Humanity May 2017 – 2020

- Worked side-by-side with Habitat Wake staff, partner families, and community partners to build new homes for our neighborhood.

Departmental Recruiting Captain Jan. 2017 – Apr. 2017

- Collaborated with other eight students in the team organizing a four-day visit for more than 30 domestic Ph.D. recruits to our department at NCSU during the recruiting weekend; hit the record of 65% acceptance from the people who visited.

PRESENTATIONS

Invited Talks:

7. "Integrated Computational Engineering Towards Accelerated Screening and Optimization for Nanoporous Materials", *EFRC-Hub-CMS-CCS Virtual Principal Investigators' Meeting*, Virtual, Oct. 2021. **(DOE Team Science Contest Winner Talk)**
6. "Can We Define a Unique Microscopic Pressure in Inhomogeneous Fluids?", *The 2nd Meeting of the Special Interest Group in Non-Equilibrium Molecular Dynamics*, UK Fluids Network, Virtual, Sept. 2021 (video).
5. "Pressure Tensor at Nanoscale: Theory, Applications and Challenges", *ATOMS Virtual Seminar Series*, Universidade Federal do Rio de Janeiro, Brazil, Virtual, June 2021 (video).
4. "Can We Define a Unique Microscopic Pressure in Inhomogeneous Fluids?", *Statistical Thermodynamics and Molecular Simulations (STMS) Seminar Series,* Virtual, Dec. 2020.
3. "Conformal Sites Theory and High-Pressure Phenomena in Adsorbed Films", *Northwestern University*, Evanston, IL, USA, Dec. 2019.
2. "High Pressure Phenomena in Adsorbed Films: A '2D Route' to the Effective Tangential Pressure", *Zhejiang University*, Hangzhou, China, Dec. 2018.
1. "High Pressure Phenomena in Adsorbed Films: A '2D Route' to the Effective Tangential Pressure", *Invited Talk Series in State Key Laboratory of Chemical Engineering at ECUST*, Shanghai, China, Dec. 2018.

Oral Talks:

16. "Energy Fingerprints for Machine Learning Prediction of Adsorption in Nanoporous Materials", *AIChE Annual Meeting*, Phoenix, AZ, USA, Nov. 2022.
15. "Two-dimensional Energy Histograms as Features for Machine Learning to Predict Adsorption in Diverse Nanoporous Materials", *14th International Conference on Fundamentals of Adsorption (FOA14)*, Broomfield, CO, USA, May 2022.
14. "Two-dimensional Energy Histograms as Features for Machine Learning to Predict Adsorption in Diverse Nanoporous Materials", *AIChE Annual Meeting*, Boston, MA, USA, Nov. 2021.
13. "Two-dimensional Energy Histograms as Features for Machine Learning to Predict Adsorption in Diverse Nanoporous Materials", *Nanoporous Materials Genome Center (NMGC) All-Hands Meeting*, Virtual, Sept. 2021.
12. "Two-Dimensional Energy Histograms as Features for Machine Learning to Predict Adsorption in Metal-Organic Frameworks", *Midwest Thermodynamics and Statistical Mechanics Conference*, Virtual, June 2021.
11. "Can We Define a Unique Microscopic Pressure in Inhomogeneous Fluids?", *AIChE Annual Meeting*, Virtual, Nov. 2020.
10. "Next-generation High-pressure Manufacturing: Defining and Understanding the Pressure Tensor in Thin Adsorbed Films", *Schoenborn Graduate Research Symposium*, NCSU, Raleigh, NC, USA, Jan. 2020.
9. "Thermodynamics in Reduced Dimensionalities", *AIChE Annual Meeting*, Orlando, FL, USA, Nov. 2019.
8. "Bottom-up Approach to the Coarse-grained Surface Model: Effective Solid-Fluid Potentials for Adsorption on Heterogeneous Surfaces", *AIChE Annual Meeting*, Orlando, FL, USA, Nov. 2019.
7. "High-Pressure Phenomena in Adsorbed Films: A New Route to an Experimental Determination of Effective Tangential Pressure", *Thermodynamics 2019*, Punta Umbría, Huelva, Spain, June 2019.
6. "A '2D Route' to the Effective Tangential Pressure in Adsorbed Films: High-Density Equation of State for a Two-Dimensional Lennard-Jones Solid", *AIChE Annual Meeting*, Pittsburgh, PA, USA, Nov. 2018.

5. "Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface", *AIChE Annual Meeting*, Minneapolis, MN, USA, Nov. 2017.
4. "Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface", *International Research & Training Group (IRTG) 1524 Annual Meeting*, Raleigh, NC, USA, Oct. 2017.
3. "Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface", *Thermodynamics 2017*, Edinburgh, United Kingdom, Sept. 2017.
2. "Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface", *International Workshop on Mesoscale Theory and Simulation for Interfacial Problems*, ECUST, Shanghai, China, June 2017.
1. "Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface", *IRTG 1524 Annual Meeting*, Neuruppin, Germany, Oct. 2016.

Posters:

13. "Nanoporous Materials for Energy, Healthcare, and Sustainability", *AIChE Annual Meeting*, Phoenix, AZ, USA, Nov. 2022.
12. "Computational Engineering Towards the Transformation of Energy-Intensive Processes", *AIChE Annual Meeting*, Boston, MA, USA, Nov. 2021.
11. "MOFDB: An Accessible Online Database of Computational Adsorption Data for Nanoporous Materials", *NMGC All-Hands Meeting*, Virtual, Oct. 2020.
10. "High-Pressure Phenomena in Adsorbed Films: A New Route to an Experimental Determination of Effective Tangential Pressure", *AIChE Annual Meeting*, Orlando, FL, USA, Nov. 2019.
9. "A '2D Route' to the Effective Tangential Pressure in Adsorbed Films: High-Density Equation of State for a Two-Dimensional Lennard-Jones Solid", *Thermodynamics 2019*, Punta Umbría, Huelva, Spain, June 2019.
8. "Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surfaces", *AIChE Annual Meeting*, Pittsburgh, PA, USA, Oct. 2018.
7. "A '2D Route' to the Effective Tangential Pressure in Adsorbed Films: High-Density Equation of State for a Two-Dimensional Lennard-Jones Solid", *Foundations of Molecular Modeling and Simulation (FOMMS)*, Delavan, WI, USA, July 2018. **(Best Poster Award)**
6. "Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surfaces", *8th International Workshop on Characterization of Porous Materials (CPM8)*, Delray Beach, FL, USA, May 2018. **(Best Poster Award)**
5. "High-density Equation of State for a Two-Dimensional Lennard-Jones Solid", *Schoenborn Graduate Research Symposium*, NCSU, Raleigh, NC, USA, Jan. 2018.
4. "Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surfaces", *Symposium on Molecular Theory and Modeling: In Honor of the 80th birthday of Professor Keith E. Gubbins*, Raleigh, NC, USA, May 2017.
3. "Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface", *IRTG 1524 Spring School: Self-Assembly in Soft Matter Systems*, Beverly, MA, USA, Mar. 2017.
2. "Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface", *Schoenborn Graduate Research Symposium*, NCSU, Raleigh, NC, USA, Jan. 2017.
1. "Effect of Non-ionic Surfactants on the Extraction of Caprolactam from Benzene Using Water", *SciMeeting - Multiscale Modeling & Simulation for Product and Process Design*, Dalian, China, Sept. 2014.