KAIHANG SHI

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EDUCATION

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

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

PROFESSIONAL EXPERIENCE

Tenure-track Assistant Professor — Aug. 2023 – present
in Chemical and Biological Engineering, University at Buffalo – SUNY, Buffalo, NY

Postdoctoral Scholar — Aug. 2020 – Aug. 2023
in Chemical and Biological Engineering, Northwestern University, Evanston, IL

Graduate Research Assistant — Aug. 2015 – July 2020
in Chemical and Biomolecular Engineering, NCSU, Raleigh, NC

Undergraduate Research Assistant — Aug. 2013 – Aug. 2015
in State Key Laboratory of Chemical Engineering, ECUST, Shanghai, China

HONORS AND AWARDS

Academic Awards

2021 **DOE Team Science Contest Winner (Team Leader)**, US Department of Energy (DOE).
2020 **James K. Ferrell Outstanding Ph.D. Graduate Award**, NCSU.
2019 **AIChE CoMSEF Graduate Student Award**, American Institute of Chemical Engineers (AIChE).
2018 **FOMMS Poster Prize**, Foundations of Molecular Modeling and Simulation (FOMMS) Meeting.
2018 **Outstanding Poster Prize**, 8th International Workshop on Characterization of Porous Materials.
2014 **Cheng Siwei Chancellor's Fellowship**, ECUST.
2014 **Special Prize for Academic Excellence (Top 1%)**, ECUST.

Teaching Awards

2016 – 2018 **Mentored Teaching Fellowships (×3)**, NCSU.
2016 Fall **Linde Exceptional Teaching Assistant Award**, NCSU.

Travel Grants

2022 **FOA14 Travel Award**, 14th International Conference on Fundamentals of Adsorption.
2019 Spring **Graduate Student Association Travel Assistance Award**, NCSU.
2018 **NSF Travel Award**, 8th International Workshop on Characterization of Porous Materials.

TEACHING EXPERIENCE

University at Buffalo
Lecturer, CE 525 Advanced Chemical Engineering Thermodynamics — 2023 Fall

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

NCSU

Guest Lecturer, CHE 315 Undergraduate Thermo I	2020 Spring
Guest Lecturer, CHE 713 Graduate Thermodynamics	2016 – 2019 Fall
Guest Lecturer, CHE 775 Multi-Scale Modeling of Matter	2019 Spring
Teaching Assistant, CHE 713 Graduate Thermodynamics	2016 – 2018 Fall
Teaching Assistant, CHE 331 Chemical Engineering Lab II	2016 Spring

PUBLICATIONS

Double dagger (‡) denotes equal contribution. Asterisk (*) denotes corresponding authors. Google Scholar

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

19. R. Wang‡, **K. Shi**‡, J. Liu, R.Q. Snurr*, and J.T. Hupp*, "Water-Accelerated Transport: Vapor-Phase Nerve Agent Simulant Delivery within a Catalytic Zirconium Metal–Organic Framework as a Function of Relative Humidity", *Journal of the American Chemical Society,* 145 (2023): 13979–13988.
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. (**Journal cover**).
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, 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.

MENTORING EXPERIENCE

Undergraduate Students

Priyen Shah (Northwestern University, now Master's student at UCLA)	Summer 2022
Julia Merlin (CoMSEF Scholars REU Program, Georgia Tech)	Summer 2021
Zongwei Huang (NCSU, now Ph.D. student at the University of Michigan)	Summer 2018-2019
Shicheng Li (NCSU)	Summer 2018
Kai Gu (NCSU, now Ph.D. student at the University of Toronto)	Summer 2017
Yifan Shen (NCSU, now Deep Learning Software Engineer at Apple)	Summer 2017

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 >45 manuscripts for a total of 20 professional journals, including *Advanced Science*, *npj Computational Materials*, *Journal of Chemical Physics*, *Journal of Physical Chemistry A/B/C/Letters*, *Chemical Science*, *Journal of Colloid and Interface Science*, *Inorganic Chemistry Frontiers*, *New Journal of Physics*, *Journal of Computational Physics*.

Conference

- Chair, "Invited sessions in honor of Keith Gubbins' 85th birthday", AIChE Annual Meeting, Phoenix, AZ, USA, 2022.
- Poster Judge, 14th International Conference on Fundamentals of Adsorption, USA, 2022.
- Co-Chair, "Applications of Molecular Modeling to Study Interfacial Phenomena" and "Molecular Simulation and Modeling of Complex Molecules", AIChE Annual Meeting, Boston, MA, USA, 2021.

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.

PROFESSIONAL AFFILIATIONS

- Member, American Institute of Chemical Engineers (AIChE) 2017 – present
- Member, American Association for the Advancement of Science (AAAS) 2021 – present
- Member, The International Adsorption Society 2022 – present