

# KAIHANG SHI

Department of Chemical & Biological Engineering  
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## EDUCATION

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- Ph.D.** North Carolina State University (NCSU), Raleigh, NC, USA 2020  
in Chemical and Biomolecular Engineering  
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

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- Postdoctoral Scholar**, Northwestern University, Evanston, IL, USA Aug. 2020 – present  
in Chemical and Biological Engineering with Randall Snurr
- Developed physics-inspired features for machine learning to predict adsorption of complex molecules in diverse nanoporous materials.
  - Co-led the development and management of a first-of-its-kind, online adsorption database “[MOFDB](#)”.
- 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 an experimentally friendly ‘2D-route’ to the effective tangential pressure in thin adsorbed films, using an accurate two-dimensional 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 industrial extraction process for caprolactam, adsorption dynamics of triblock copolymers, and the formation of polycation/DNA-like complex.

## TEACHING EXPERIENCE

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- Invited Lecturer**, 12/24-623 Molecular Simulation of Materials, Carnegie Mellon University 2020 Fall
- Presented **one** invited 110-minute lecture on microscopic pressure tensor.
- Guest Lecturer**, CHE315 Undergraduate Thermo I, NCSU 2020 Spring
- Presented **three** independent 50-minute lectures on classical thermodynamics.
- Guest Lecturer**, CHE713 Graduate Thermodynamics, NCSU 2016 – 2019 Fall
- Presented **eighteen** independent 75-minute lectures on classical thermodynamics and on 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 **one** 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 the best TA I’ve ever had. He’s always very open to questions and he will grind through questions.* 3). *Kaihang was excellent at teaching and explaining the material.* 4). *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

## HONORS AND AWARDS

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- 2021**      **Student and Postdoc Team Science Contest Winner (Team leader)**, “Integrated Computational Engineering Towards Accelerated Screening and Optimization for Nanoporous Materials” presented at 2021 EFRC-Hub-CMS-CCS Virtual Principal Investigators’ Meeting, The U.S. Department of Energy’s Office of Basic Energy Sciences.
- 2020**      **James K. Ferrell Outstanding Ph.D. Graduate Award**, I was invited to give a speech at the [2021 Spring Commencement Ceremony](#) for the Department of Chemical and Biomolecular Engineering, NCSU.
- 2019**      **AIChE’s CoMSEF Graduate Student Award**, distinguished national research award presented by *The Computational Molecular Science and Engineering Forum (CoMSEF)* at the *American Institute of Chemical Engineers (AIChE) Annual Meeting*, Orlando, FL, USA.
- 2019 Spring**      **GSA Travel Assistance Award**, The Graduate Student Association, NCSU.
- 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.
- 2018**      **NSF Travel Award**, *CPM8*, Delray Beach, FL, USA.
- 2016 – 2018**      **Mentored Teaching Fellowships (×3)**, awarded to ten outstanding graduate students in teaching per semester across the entire College of Engineering, NCSU.
- 2016 Fall**      **Praxair Exceptional Teaching Assistant Award**, only one recipient department-wide per semester, Praxair, Inc. & NCSU.
- 2014**      **Cheng Siwei Chancellor’s Fellowship**, the most prestigious university-wide award, ECUST.
- 2014**      **Honorable Mention**, Mathematical Contest in Modeling, USA.
- 2014**      **Special Prize for Academic Excellence (Top 1%)**, ECUST.

## TRAINING IN PROPOSAL WRITING

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**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 (Pending, 2021). Contributions: Led writing two sections of 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 6,020,000 CPU hours, 2021-2022). Contributions: 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 (Returned without review, 2018). Contributions: Prepared figures and assisted with assembling the proposal.

## PUBLICATIONS

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**15 peer-reviewed papers | 1 book chapter | 4 papers in draft/to be submitted**

Work published: **7 × 1st author | 5 × 2nd author | 3 × corresponding author**

(“\*” Indicates authors contributed equally; “#” Indicates corresponding authors)

### Book Chapter

1. **K. Shi**<sup>#</sup>, 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. [\[link\]](#)

### Journal Publications

19. A. Furuse, R. Futamura, **K. Shi**, Y. Shen, K.E. Gubbins, K. Kaneko<sup>#</sup>, “High Pressure Organic Reaction through In-Pore Superhigh Pressure Effect of SWCNTs”, 2021, *in draft*.

18. **K. Shi**, Z. Li, D.M. Anstine, D. Tang, C.M. Colina, D.S. Sholl, J.I. Siepmann, and R.Q. Snurr<sup>#</sup>, “Two-dimensional Energy Histograms as Features for Machine Learning to Predict Adsorption in Diverse Nanoporous Materials”, 2021, *in draft, manuscript available upon request*.
17. P. Montero de Hijes, **K. Shi**, E. Sanz, C. Vega<sup>#</sup>, “Stabilization of the Ice Critical Nuclei”, 2021, *in draft*.
16. N.S. Bobbitt, **K. Shi**, B.J. Bucior, H. Chen, N. Tracy-Amoroso, Z. Li, D. Siderius, R.Q. Snurr<sup>#</sup>, “MOFdb: An Accessible Online Database of Computational Adsorption Data for Nanoporous Materials”, 2021, *in draft*.
15. **K. Shi**<sup>#</sup>, E.E. Santiso<sup>#</sup>, K.E. Gubbins<sup>#</sup>, “Can We Define a Unique Microscopic Pressure in Inhomogeneous Fluids?”, *Journal of Chemical Physics*, 154 (2021): 084502. [\[link\]](#)
14. P. Montero de Hijes, **K. Shi**, E.G. Noya, E.E. Santiso, K.E. Gubbins, E. Sanz, C. Vega<sup>#</sup>, “The Young-Laplace Equation for a Solid-Liquid Interface”, *Journal of Chemical Physics*, 153 (2020): 191102. [\[link\]](#)
13. **K. Shi**<sup>#</sup>, Y. Shen, E.E. Santiso<sup>#</sup>, K.E. Gubbins<sup>#</sup>, “Microscopic Pressure Tensor in Cylindrical Geometry: Pressure of Water in a Carbon Nanotube”, *Journal of Chemical Theory and Computation*, 16 (2020): 5548-5561. [\[link\]](#)
12. S. Wang, **K. Shi**, A. Tripathi, U. Chakraborty, G.N. Parsons<sup>#</sup>, S.A. Khan<sup>#</sup>, “Designing PIM-1 Microfibers with Tunable Morphology and Porosity via Controlling Solvent/Nonsolvent/Polymer Interactions”, *ACS Applied Polymer Materials*, 2 (2020): 2434-2443. [\[link\]](#)
11. Y. Long, J.C. Palmer<sup>#</sup>, B. Coasne<sup>#</sup>, **K. Shi**, M. Sliwinska-Bartkowiak, K.E. Gubbins<sup>#</sup>, “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. [\[link\]](#)
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<sup>#</sup>, S. Menegatti<sup>#</sup>, “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. [\[link\]](#)
9. **K. Shi**, E.E. Santiso<sup>#</sup>, K.E. Gubbins<sup>#</sup>, “Conformal Sites Theory for Adsorbed Films on Energetically Heterogeneous Surfaces”, *Langmuir*, 36 (2020): 1822–1838. [\[link\]](#)
8. Z. Dai, D.T. Lee, **K. Shi**, S. Wang, H.F. Barton, J. Zhu, J. Yan, Q. Ke<sup>#</sup>, G.N. Parsons<sup>#</sup>, “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. [\[link\]](#)
7. C. Cutright, Z. Brotherton, L. Alexander, J. Harris, **K. Shi**, S. Khan, J. Genzer, S. Menegatti<sup>#</sup>, “Packing Density, Homogeneity, and Regularity: Quantitative Correlations between Topology and Thermoresponsive Morphology of PNIPAM-co-PAA Microgel Coatings”, *Applied Surface Science*, 508 (2020): 145129. [\[link\]](#)
6. **K. Shi**, E.E. Santiso<sup>#</sup>, K.E. Gubbins<sup>#</sup>, “Bottom-Up Approach to the Coarse-Grained Surface Model: Effective Solid–Fluid Potentials for Adsorption on Heterogeneous Surfaces”, *Langmuir*, 35 (2019): 5975–5986. [\[link\]](#)
5. K.E. Gubbins<sup>#</sup>, K. Gu, L. Huang<sup>#</sup>, Y. Long, J.M. Mansell, E.E. Santiso<sup>#</sup>, **K. Shi**, M. Śliwińska-Bartkowiak, D. Srivastava, “Surface-Driven High-Pressure Processing”, *Engineering*, 4 (2018): 311–320. Special issue on Green Industrial Processes. [\[link\]](#)
4. **K. Shi**<sup>\*</sup>, K. Gu<sup>\*</sup>, Y. Shen, D. Srivastava, E.E. Santiso<sup>#</sup>, K.E. Gubbins<sup>#</sup>, “High-Density Equation of State for a Two-Dimensional Lennard-Jones Solid”, *Journal of Chemical Physics*, 148 (2018): 174505. [\[link\]](#)
3. Y. Xu, **K. Shi**, S. Zhao<sup>#</sup>, X. Guo, J. Wang<sup>#</sup>, “Block Length Determines the Adsorption Dynamics Mode of Triblock Copolymers to a Hydrophobic Surface”, *Chemical Engineering Science*, 142 (2016): 180–189. [\[link\]](#)
2. B. Zhan, **K. Shi**, Z. Dong, W. Lv, S. Zhao<sup>#</sup>, X. Han<sup>#</sup>, H. Wang, H. Liu, “Coarse-Grained Simulation of Polycation/DNA-Like Complexes: Role of Neutral Block”, *Molecular Pharmaceutics*, 12 (2015): 2834-2844. [\[link\]](#)
1. **K. Shi**, C. Lian, Z. Bai, S. Zhao<sup>#</sup>, 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. [\[link\]](#)

21 conference/seminars talks | 12 posters | 5 invited talks | 6 overseas talks | 2 best poster awards

Oral:

21. **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”, *2021 AIChE Annual Meeting*, Boston, MA, USA, Nov. 8, 2021.
20. **K. Shi**, Y. Sun, J.I. Siepmann, and R.Q. Snurr, “Integrated Computational Engineering Towards Accelerated Screening and Optimization for Nanoporous Materials”, *2021 EFRC-Hub-CMS-CCS Virtual Principal Investigators’ Meeting*, Virtual, Oct. 19, 2021. **(Team Science Contest Winner Talk)**
19. **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”, *Nanoporous Materials Genome Center (NMGC) 2021 All-Hands Meeting*, Virtual, Sept. 13, 2021.
18. **K. Shi**, E.E. Santiso, K.E. Gubbins, “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. 6, 2021. Recorded video is available [here](#). **(Invited Talk)**
17. **K. Shi**, “Pressure Tensor at Nanoscale: Theory, Applications and Challenges”, *ATOMS Virtual Seminar Series*, Universidade Federal do Rio de Janeiro, Brazil, Virtual, June 24, 2021. Recorded video is available [here](#). **(Invited Talk)**
16. **K. Shi**, Z. Li, R.Q. Snurr, “Two-Dimensional Energy Histograms as Features for Machine Learning to Predict Adsorption in Metal-Organic Frameworks”, *2021 Midwest Thermodynamics and Statistical Mechanics Conference*, Virtual, June 16, 2021.
15. **K. Shi**, E.E. Santiso, K.E. Gubbins, “Can We Define a Unique Microscopic Pressure in Inhomogeneous Fluids?”, *Statistical Thermodynamics and Molecular Simulations (STMS) Seminar Series*, Virtual, Dec. 18, 2020. **(Invited Talk)**
14. **K. Shi**, E.E. Santiso, K.E. Gubbins, “Can We Define a Unique Microscopic Pressure in Inhomogeneous Fluids?”, *2020 AIChE Annual Meeting*, Virtual, Nov. 17, 2020.
13. **K. Shi**, E.E. Santiso, K.E. Gubbins, “Next-generation High-pressure Manufacturing: Defining and Understanding the Pressure Tensor in Thin Adsorbed Films”, *Schoenborn Graduate Research Symposium*, NCSU, Raleigh, NC, USA, Jan. 27, 2020.
12. **K. Shi**, E.E. Santiso, K.E. Gubbins, “Conformal Sites Theory and High-Pressure Phenomena in Adsorbed Films”, *Northwestern University*, Evanston, IL, USA, Dec. 11, 2019.
11. **K. Shi**, J.M. Mansell, E.E. Santiso, K.E. Gubbins, “Thermodynamics in Reduced Dimensionalities”, *2019 AIChE Annual Meeting*, Orlando, FL, USA, Nov. 14, 2019.
10. **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”, *2019 AIChE Annual Meeting*, Orlando, FL, USA, Nov. 12, 2019.
9. **K. Shi**, E.E. Santiso, K.E. Gubbins, “High-Pressure Phenomena in Adsorbed Films: A New Route to an Experimental Determination of Effective Tangential Pressure”, *Thermodynamics 2019*, Punta Umbría, Huelva, Spain, June 27, 2019.
8. **K. Shi**, E.E. Santiso, K.E. Gubbins, “High Pressure Phenomena in Adsorbed Films: A ‘2D Route’ to the Effective Tangential Pressure”, *Zhejiang University*, Hangzhou, China, Dec. 14, 2018. **(Invited Talk)**
7. **K. Shi**, E.E. Santiso, K.E. Gubbins, “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 East China University of Science & Technology*, Shanghai, China, Dec. 12, 2018. **(Invited Talk)**
6. **K. Shi**, K. Gu, Y. Shen, D. Srivastava, E.E. Santiso, K.E. Gubbins, “A ‘2D Route’ to the Effective Tangential Pressure in Adsorbed Films: High-Density Equation of State for a Two-Dimensional Lennard-Jones Solid”, *2018 AIChE Annual Meeting*, Pittsburgh, PA, USA, Nov. 1, 2018.
5. **K. Shi**, E.E. Santiso, K.E. Gubbins, “Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface”, *2017 AIChE Annual Meeting*, Minneapolis, MN, USA, Nov. 2, 2017.
4. **K. Shi**, E.E. Santiso, K.E. Gubbins, “Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface”, *International Research & Training Group (IRTG) 1524 Annual Meeting 2017*, Raleigh, NC, USA, Oct. 7, 2017.

3. **K. Shi**, E.E. Santiso, K.E. Gubbins, “Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface”, *Thermodynamics 2017*, Edinburgh, United Kingdom, Sept. 6, 2017.
2. **K. Shi**, E.E. Santiso, K.E. Gubbins, “Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface”, *International Workshop on Mesoscale Theory and Simulation for Interfacial Problems*, East China University of Science & Technology, Shanghai, China, June 10, 2017.
1. **K. Shi**, K.E. Gubbins, “Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface”, *International Research & Training Group (IRTG) 1524 Annual Meeting 2016*, Neuruppin, Germany, Oct. 10, 2016.

**Poster:**

12. **K. Shi**, “Computational Engineering Towards the Transformation of Energy-Intensive Processes”, *2021 AIChE Annual Meeting*, Boston, MA, USA, Nov. 7, 2021.
11. **K. Shi**, N.S. Bobbitt, B.J. Bucior, H. Chen, N. Tracy-Amoroso, Z. Li, D. Siderius, R.Q. Snurr, “MOFdb: An Accessible Online Database of Computational Adsorption Data for Nanoporous Materials”, *NMGC 2020 All-Hands Meeting*, Virtual, Oct. 9, 2020.
10. **K. Shi**, E.E. Santiso, K.E. Gubbins, “High-Pressure Phenomena in Adsorbed Films: A New Route to an Experimental Determination of Effective Tangential Pressure”, *2019 AIChE Annual Meeting*, Orlando, FL, USA, Nov. 12, 2019.
9. **K. Shi**, K. Gu, Y. Shen, D. Srivastava, E.E. Santiso, K.E. Gubbins, “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 28, 2019.
8. **K. Shi**, E.E. Santiso, K.E. Gubbins, “Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surfaces”, *2018 AIChE Annual Meeting*, Pittsburgh, PA, USA, Oct. 29, 2018.
7. **K. Shi**, K. Gu, Y. Shen, D. Srivastava, E.E. Santiso, K.E. Gubbins, “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 2018)*, Delavan, WI, USA, July 18, 2018. (**Best Poster Award**)
6. **K. Shi**, E.E. Santiso, K.E. Gubbins, “Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surfaces”, *8th International Workshop on Characterization of Porous Materials (CPM8)*, Delray Beach, FL, USA, May 7, 2018. (**Best Poster Award**)
5. **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”, *Schoenborn Graduate Research Symposium*, NCSU, Raleigh, NC, USA, Jan. 22, 2018.
4. **K. Shi**, E.E. Santiso, K.E. Gubbins, “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 1, 2017.
3. **K. Shi**, K.E. Gubbins, “Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface”, *International Research & Training Group (IRTG) 1524 Spring School 2017: Self-Assembly in Soft Matter Systems*, Beverly, MA, USA, Mar. 7, 2017.
2. **K. Shi**, K.E. Gubbins, “Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surface”, *Schoenborn Graduate Research Symposium*, NCSU, Raleigh, NC, USA, Jan. 23, 2017.
1. **K. Shi**, C. Lian, Z. Bai, S. Zhao, H. Liu, “Effect of Non-ionic Surfactants on the Extraction of Caprolactam from Benzene Using Water”, *SciMeeting2014–Multiscale Modeling & Simulation for Product and Process Design*, Dalian, China, Sept. 12, 2014.

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## MENTORING EXPERIENCE

### Northwestern University

Mentored **1** undergraduate student: Julia Merlin (through CoMSEF Scholars REU Program, Summer 2021, undergraduate student from Georgia Tech).

- Culminated with one paper in preparation.

### 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

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- **Department of Energy (DOE) Basic Energy Sciences (BES) Early Career Network (ECN) Representative**, Nanoporous Materials Genome Center (NMGC), serve as the liaison between NMGC members and the DOE BES ECN, and is leading the organization of invited webinars on grant writing, Oct. 2021 – Present.
- **Proposal Reviewer**, DOE Office of Science Graduate Student Research (SCGSR) program.
- **Journal Referee**, serving as the referee for a total of 11 professional journals, including *Journal of Physical Chemistry Letters*, *Journal of Chemical Physics*, *New Journal of Physics*, *Molecular Physics*, *Journal of Computational Physics*, *Nanoscale Research Letter*, *RSC Advances*.
- **Conference Co-Chair**, 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**, worked side-by-side with Habitat Wake staff, partner families, and community partners to build new homes for our neighborhood, May 2017 – 2020.
- **Recruiting Captain**, 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 North Carolina State University during the recruiting weekend; Hit the record of 65% acceptance from the people who visited, Jan. 2017 – Apr. 2017.

## REFERENCES

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*Additional contact details and references are available upon request.*

### **Prof. Keith E. Gubbins**

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