Qing Shao (qshao@uky.edu) https://www.shaoresearch.com/
159 FPAT, University of Kentucky, Lexington, KY 40506

Education

2000-2004	Nanjing University of Technology, China, Chemical Engineering Bachelor
2004-2009	Nanjing University of Technology, China, Chemical Engineering PhD program
2009-2014	University of Washington, Seattle, Chemical Engineering Ph.D.

Research Interests

Computation-driven Materials Design
Interfacial Thermodynamics
Peptide Assembly
Artificial Intelligence
Biomaterials

Research Experience

2018-current Assistant Professor Department of Chemical and Materials Engineering, University of Kentucky

2014-2018 Postdoctoral Research Scholar Department of Chemical and Biomolecular Engineering, North Carolina State University, Supervisor: Prof. Carol K. Hall

1. Developed coarse-grained models for protein-protein and protein-nanoparticle interactions
2. Investigated adsorption isotherms of proteins on nanoparticles
3. Investigated allosteric effects of nanoparticles on proteins
4. Developed computational models that can predict protein-nanoparticle interaction energy
5. Investigated co-assembling peptides
6. Investigated lyophilization processes

2009-2014 Department of Chemical Engineering, University of Washington,
Supervisor: Prof. Shaoyi Jiang

1. Developed force field parameters for zwitterionic molecules
2. Investigated hydration, ion interactions and self-associations of zwitterionic molecules
3. Design zwitterionic anti-biofouling materials

2004-2009 State Key Laboratory of Material-oriented Chemical Engineering, Nanjing University of Technology, Supervisor: Prof. Xiaohua Lu

1. Studied structural properties of ethanol molecules in carbon nanotube pores
2. Investigated ionic hydration carbon nanotube pores

Teaching

2019 Fall CHE415 Separation Processes
2018 Fall CHE415 Separation Processes
2018 Winter CHE220 Computational tools in chemical engineering

Service

Co-Chair of the "Data-driven design and modeling of biomaterials" session for AIChE annual meeting (2019-)
Co-chair the "Modeling of Biomaterials" Session in the AIChE annual meetings 2015-2018

Awards

2015-16 Professional Development Award for Postdocs, North Carolina State University

Professional Memberships/Affiliations

American Institute of Chemical Engineers

Publication List (h-index: 25 from Google Scholar)

Google Scholar profile:
https://scholar.google.com/citations?hl=en&user=LOW5pcEAAAAJ&view_op=list_works

At Kentucky

(1) Seroski, D.T., Dong, X., Wong, K.M., Liu, R., **Shao, Q**., Paravastu, A.K., Hall, C.K. and Hudalla, G.A., 2020. Charge guides pathway selection in β-sheet fibrillizing peptide co-assembly. Communications Chemistry, 3, 1-11.

(2) Xu N., Shi Y, He Y*, and **Shao Q***. A Deep-Learning Potential for Crystalline and Amorphous Li-Si Alloys, *J. Phys. Chem. C*, 2020, 124, 12678-12688

(3) **Shao Q*** Effect of Conjugated $(EK)_{10}$ Peptide on Structural and Dynamic Properties of Ubiquitin Protein: a Molecular Dynamics Simulation Study, *J. Mater. Chem. B*, 2020, 8, 6934-6943

(4) Nguyen, M. T, **Shao Q*** Effects of zwitterionic molecules on ionic association in ethylene oxide-based electrolytes, *Fluid Phase Equil.* 2020, 515, 112572

(5) Nguyen, M. T, **Shao Q***. Effect of Zwitterionic Molecules on Ionic Transport under Electric Fields: A Molecular Simulation Study, *J. Chem. Eng. Data*, 2020, 65, 2, 385–395

(6) **Qing Shao**, Kong, M. Wong, Dillon T. Seroski, Yiming Wang, Renjie Liu, Anant K. Paravastu, Gregory A. Hudalla, and Carol K. Hall, Anatomy of a Selectively Co-assembled β-sheet Peptide Nanofiber, Proc. Natl. Acad. Sci. U.S.A. 2020, 117, 4710-4717

(7) **Shao Q**.; A computational avenue towards understanding and design of zwitterionic anti-biofouling materials *Mol. Simul*. 2019, 1-12.

Before Kentucky

(1) Han X, Leng C., **Shao Q**, Jiang S. Y., Chen Z, Absolute Orientations of Water Molecules at Zwitterionic Polymer Interfaces and Interfacial Dynamics after Salt Exposure Langmuir, 2019, 355, 1327-1334

(2) **Shao Q.;** Hall C. K., Selectivity of Glycine for Facets on Gold Nanoparticles J. Phys. Chem. B, 2017, 122, 13, 3491-3499

(3) **Shao Q.;** Hall C. K., Allosteric Effects of Gold Nanoparticle on Human Serum Albumin, *Nanoscale* 2017, 9(1):380-390

(4) **Shao Q.;** Hall C. K., Binding Preferences of Amino Acids for Gold Nanoparticles: a Molecular Simulation Study. *Langmuir* 2016, 32(31):7888-7896

(5) **Shao Q.;** Hall C. K., Protein Adsorption on Nanoparticles: Model Development Using Computer Simulation *J. Phys. Conden. Matter*. 2016 28(41):414019

(6) **Shao Q.;** Hall C. K., A Discontinuous-Potential Model for Protein-Protein Interactions, *Molecular Modeling and Simulation: Applications and Perspectives* 2016:1-20

(7) Wang Y. M., **Shao Q.,** and Hall C. K., N-terminal Prion Protein Peptides (PrP120-144) Form Parallel In-register β-sheets via Multiple Nucleation-dependent Pathways, *J. Biol. Chem.* 291(42):22093-22105.

(8) Zhao, Y.; Bai, T., **Shao, Q.**, Jiang, S. Y., Shen Q. A., Thermoresponsive self-assembled NiPAm-zwitterion copolymers, *Polym. Chem.*, 2015, 6, 1066-1077.

(9) **Shao, Q.;** Jiang, S. Y., Molecular Understanding and Design of Zwitterionic Materials. *Adv. Mater.* 2015,27(1):15-26.

(10) **Shao, Q.;** Jiang, S. Y., Influence of Charged Groups on Properties of Zwitterionic Moieties: A Molecular Simulation Study. *J. Phys. Chem. B*, 2014, 118 (27): 7630–7637.

(11) **Shao, Q.;** Mi L., Bai T., Han X., Liu S., Li Y. T.; and Jiang S. Y., Differences in Cationic and Anionic Charge Densities Dictate Zwitterionic Associations and Stimuli Responses. *J. Phys. Chem. B*, 2014, 118 (24): 6956–6962.

(12) **Shao, Q.;** White, A. D.; Jiang, S. Y., Difference of Carboxybetaine and Oligo(ethylene glycol) Moieties in Altering Hydrophobic Interactions: A Molecular Simulation Study. *J. Phys. Chem. B*, 2014, 118(1): 189-194.

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(14) Mi L.; White A. D.; **Shao Q.;** Setlow P.; Li Y. Q.; Jiang S. Y.; Chemical Insights into Dodecylamine Spore Lethal Germination. *Chem. Sci.* 2014, 5, 3320-3324.
(15) Leng C.; Han, X. F.; **Shao, Q.;** Zhu, Y. H.; Li, Y. T.; Jiang, S. Y.; Chen, Z. *In situ* Probing the Surface Hydration of Zwitterionic Polymer Brushes: Structural and Environmental Effects. *J. Phys. Chem. C*, 2014, 118 (29): 15840–15845.
(16) Sundaram, H. S.; Ella-Menye, J. R.; Brault N. D.; **Shao Q.**; Jiang S. Y., Reversibly Switchable Polymer with Cationic/Zwitterionic/Anionic Behavior through Synergistic Protonation and Deprotonation. *Chem. Sci.*, 2014, 5(1): 200-205.
(17) **Shao, Q.;** Jiang, S. Y., Effects of Carbon Spacer Length on Zwitterionic Carboxybetaines. *J. Phys. Chem. B*, 2013,117 (5): 1357–1366.
(18) White, A. D.; Keefe, A. J.; Ella-Menye, J.-R.; Nowinski, A. K.; **Shao, Q.;** Pfaendtner, J.; Jiang, S., Free Energy of Solvated Salt Bridges: A Simulation and Experimental Study. *J. Phys. Chem. B*, 2013, 117 (24): 7254-7259.
(19) White, A. D.; Keefe, A. J.; Nowinski, A. K.; **Shao, Q.;** Caldwell, K.; Jiang, S., Standardizing and Simplifying Analysis of Peptide Library Data. *J. Chem. Inf. Model.* 2013, 53 (2): 493-499.
(20) **Shao, Q.;** He, Y.; White, A. D.; Jiang, S. Y., Different Effects of Zwitterion and Ethylene Glycol on Proteins. *J. Chem. Phys.*, 2012, 136 (22): 225101.
(21) Mi, L.; Giarmarco, M. M.; **Shao, Q.;** Jiang, S. Y., Divalent Cation-mediated Polysaccharide Interactions with Zwitterionic Surfaces. *Biomaterials* 2012, 33 (7): 2001-2006.
(22) **Shao, Q.;** He, Y.; Jiang, S. Y., Molecular Dynamics Simulation Study of Ion Interactions with Zwitterions. *J. Phys. Chem. B*, 2011, 115 (25): 8358-8363.
(23) He, Y.; **Shao, Q.;** Tsao, H. K.; Chen, S. F.; Goddard, W. A.; Jiang, S. Y., Understanding Three Hydration-Dependent Transitions of Zwitterionic Carboxybetaine Hydrogel by Molecular Dynamics Simulations. *J. Phys. Chem. B*, 2011, 115 (40): 11575-11580.
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(25) He, Y.; **Shao, Q.;** Chen, S. F.; Jiang, S. Y., Chaotrope vs. Kosmotrope: Which One Has Lower Friction? *J. Chem. Phys.* 2011, 135 (15): 154702 .
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(37) Lu, L. H.; Lu, X. H.; Chen, Y. P.; Huang, L. L.; **Shao, Q.;** Wang, Q., Monte Carlo Simulation of Adsorption of Binary and Quaternary Alkane Isomers Mixtures in Zeolites: Effect of Pore Size and Structure. *Fluid Phase Equilib.* 2007, 259 (2): 135-145.
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