

Contact/Bio	Engineering C-164 98 Brett Rd, Piscataway NJ 08854	Email: ashley.guo@rutgers.edu Homepage: https://guogroup.rutgers.edu	US Citizen
Appointments	Rutgers, The State University of New Jersey , New Brunswick NJ Assistant Professor, Department of Chemical and Biochemical Engineering		Sept 2023–
	New York University , New York NY Postdoctoral Associate, Center for Soft Matter Research, Advisor: Paul Chaikin		2020–2023
Education	University of Chicago , Chicago IL Ph.D., Molecular Engineering, Advisor: Juan de Pablo		2014–2020
	California Institute of Technology , Pasadena CA B.S., Chemical Engineering (Materials track), Advisor: Julie Kornfield		2010–2014
Fellowships, Leadership & Awards	Faculty Excellence in Teaching and Advising Award , Rutgers CBE Distinguished Young Scholar , University of Washington Chemical Engineering William Rainey Harper Dissertation Fellow , University of Chicago Chicago Center for Teaching Fellow , University of Chicago Science Communication Fellow , Museum of Science & Industry, Chicago IL Arts, Culture, & Science Initiative Graduate Fellow , University of Chicago Howard Hughes Medical Institute Teaching Fellow , Caltech Reed and Ruth Brantley Undergraduate Research Fellow , Caltech		2024 2022 2018–2019 2018–2019 2015–2017 2015–2016 2014 2012
Publications * equal contribution	<p>[10] Wilken, S.*, Guo, A.Z.*, Levine, D., Chaikin, P.M., “Dynamical Approach to the Jamming Problem”, Phys. Rev. Lett., 131, 238202 (2023). [doi:10.1103/PhysRevLett.131.238202]</p> <p>[9] Fowler, W.C., Deng, C., Griffen, G.M., Teodoro, T., Guo, A.Z., Zaiden, M., Gottlieb, M., de Pablo, J.J., Tirrell, M.V., “Harnessing Peptide Binding to Capture and Reclaim Phosphate”, J. Am. Chem. Soc., 143, 4440–4450 (2021). [doi:10.1021/jacs.1c01241]</p> <p>[8] Sevgen, E., Guo, A.Z., Sidky, H., Whitmer, J., de Pablo, J., “Combined Force-Frequency Sampling for Simulation of Systems Having Rugged Free Energy Landscapes”, J. Chem. Theory Comput., 16, 1448–1455 (2020). [doi:10.1021/acs.jctc.9b00883]</p> <p>[7] Colón, Y.J., Guo, A.Z., Antony, L.B., Hoffmann, K.Q., de Pablo, J.J., “Free Energy of Metal Organic Framework Self-Assembly”, J. Chem. Phys., 150, 104502 (2019). [doi:10.1063/1.5063588]</p> <p>[6] Guo, A.Z., Lequieu, J., de Pablo J.J., “Extracting collective motions underlying nucleosome dynamics via the diffusion map”, J. Chem. Phys., 150, 054902 (2019). [doi:10.1063/1.5063851]</p> <p>[5] Guo, A.Z., Fluitt, A.M., de Pablo, J.J., “Early-stage Human Islet Amyloid Polypeptide Aggregation: Mechanisms Behind Dimer Formation”, J. Chem. Phys., 149, 025101 (2018). [doi:10.1063/1.5033458]</p> <p>[4] Guo, A.Z.*, Sevgen, E.*, Sidky, H., Whitmer, J.K., Hubbell, J.A., de Pablo, J.J., “Adaptive enhanced sampling by force-biasing using neural networks”, J. Chem. Phys., 148, 134108 (2018). [doi:10.1063/1.5020733]</p> <p>[3] Sidky, H., Colón, Y.J., Helfferich, J., Sikora, B.J., Bezik, C., Chu, W., Giberti, F., Guo, A.Z., Jiang, X., Lequieu, J., Li, J., Moller, J., Quevillon, M.J., Rahimi, M., Ramezani-Dakhel, H., Rathee, V.S., Reid, D.R., Sevgen, E., Thapar, V., Webb, M.A., Whitmer, J.K., de Pablo, J.J., “SSAGES: Software Suite for Advanced General Ensemble Simulations”, J. Chem. Phys., 148, 044104 (2018). [doi:10.1063/1.5008853]</p> <p>[2] Sadati, M., Zhou, Y., Melchert, D., Guo, A., Martinez-Gonzalez, J.A., Roberts, T.F., Zhang, R., de Pablo, J.J., “Spherical nematic shell with prolate ellipsoidal core”, Soft Matter, 13, 7465–7472</p>		

(2017). [doi:10.1039/C7SM01403A]

[1] Zhou, Y., **Guo, A.**, Zhang, R., Armas-Perez, J.C., Martinez-González, J.A., Rahimi, M., Sadati, M., de Pablo, J.J., “Mesoscale structure of chiral nematic shells”, *Soft Matter*, 12, 8983-8989 (2016). [doi:10.1039/c6sm01284a]

Submitted &
In Preparation

- [1] **Guo, A.Z.**, Wilken, S., Levine, D., Chaikin, P.M., “Active diffusing crystals in a 2D non-equilibrium system.” *In revision, Physical Review E*. [doi:10.48550/arXiv.2512.19277]
- [2] **Guo, A.Z.**, Chang, K., Corrente, N.J., “An Information-theoretic Collective Variable for Capturing Entropy in Molecular Systems.” *In preparation*.
- [3] Gokani, M., Fea, B.Z., **Guo, A.Z.**, “Molecular Simulations for Atomic Understanding of Polypeptide-Polystyrene Binding in Water.” *In preparation*.
- [4] Corrente, N.J., Barillas, K., Brown, P.R., Buettner, H.M., **Guo, A.Z.**, Konczynski, J. Mont, A.J., Shapley, N.C., “WIP: Development of a Chemical Engineering Activity for First-Year Engineering Students.” *In preparation, ASEE*

Invited
Presentations

- [11] A Data- and Information-driven Approach for Computational Soft Materials Design, 2025
First Annual Rutgers Chemical Physics Symposium, Rutgers University–Newark
- [10] A Data- and Information-driven Approach for Computational Soft Materials Design, 2025
ACS Middle Atlantic Regional Meeting (MARM), Seton Hall University
- [9] A Data- and Information-driven Approach for Computational Soft Materials Design, 2025
University of Texas at San Antonio, Dept. of Physics and Astronomy Seminar
- [8] An Information-driven Approach to Quantifying and Controlling Emergent Order, 2023
University of British Columbia Dept. of Chemical and Biological Engineering Seminar
- [7] An Information-driven Approach to Quantifying and Controlling Emergent Order, 2023
Rensselaer Polytechnic Institute Dept. of Chemical and Biological Engineering Seminar
- [6] An Information-driven Approach to Quantifying and Controlling Emergent Order, 2023
Rutgers University Department of Chemical and Biochemical Engineering Seminar
- [5] An Information-driven Approach to Quantifying and Controlling Emergent Order, 2023
University of Washington Department of Chemical Engineering Seminar
- [4] An Information-driven Approach to Quantifying and Controlling Emergent Order, 2023
UMass Amherst Department of Polymer Science and Engineering Seminar
- [3] An Information-driven Approach to Quantifying and Controlling Emergent Order, 2022
Statistical Thermodynamics and Molecular Simulations Seminar Series, Virtual
- [2] An Information-driven Approach to Quantifying and Controlling Emergent Order, 2022
University of Washington Distinguished Young Scholars Seminar
- [1] Understanding Nucleosome Dynamics using Diffusion Maps, 2019
D.E. Shaw Research, New York NY

Contributed
Presentations

- [22] An Information-Theoretic Approach for Probing Macromolecular Phase Separation Via Data Compression. 2024
AIChE Annual Meeting, San Diego CA (Oral)
- [21] A Data- and Information-Driven Approach for Computational Soft Materials Design. 2024
5th Molecular Simulations Workshop, NJIT (Poster)
- [20] A Data- and Information-Driven Approach for Computational Soft Materials Design. 2024
FOMMS, Snowbird UT (Poster)
- [19] Random Close Packing is least random in 3D, 2023
APS March Meeting, Las Vegas NV (Oral)
- [18] An Information-Driven Approach to Quantifying and Controlling Emergent Order. 2022
AIChE Annual Meeting, Phoenix AZ (Oral)

[17] An Information-Driven Approach for Controlling Emergent Order in Soft Materials. <i>AIChE Annual Meeting, Phoenix AZ</i> (Poster)	2022
[16] An Information-driven Approach to Quantifying and Controlling Emergent Order. <i>Univ. of Washington Distinguished Young Scholars Seminar</i> (Oral)	2022
[15] Higher Dimensional Biased Random Organization <i>APS March Meeting, Chicago IL</i> (Oral)	2022
[14] Characterizing phase transitions in 2D Repulsive Random Organization <i>APS March Meeting, Virtual Talk</i> (Oral)	2021
[13] Identifying Trimerization Mechanisms of Human Islet Amyloid Polypeptide through Molecular Simulation. <i>APS March Meeting, Boston MA.</i> (Oral)	2019
[12] Nonlinear Manifold Learning of Nucleosome Dynamics from Molecular Simulation <i>AIChE Annual Meeting, Pittsburgh PA.</i> (Oral)	2018
[11] Human Islet Amyloid Polypeptide: Identifying Early-Stage Aggregation Mechanisms through Molecular Simulation. <i>EQUIFASE 2018, Córdoba, Argentina.</i> (Oral)	2018
[10] Understanding Nucleosome Dynamics using Diffusion Maps <i>Frontiers of Molecular Engineering, Chicago IL</i> (Poster, <u>Best Poster Award</u>)	2018
[9] Understanding Nucleosome Dynamics using Diffusion Maps <i>Mind Bytes Symposium, University of Chicago Research Computing Center</i> (Poster)	2018
[8] Human Islet Amyloid Polypeptide: Identifying Early-Stage Aggregation Mechanisms through Molecular Simulation. <i>Mind Bytes Symposium, University of Chicago</i> (Poster)	2018
[7] Extracting collective motions underlying nucleosome dynamics via nonlinear manifold learning. <i>APS March Meeting, Los Angeles CA.</i> (Oral)	2018
[6] Human Islet Amyloid Polypeptide: Identifying Early-Stage Aggregation Mechanisms through Molecular Simulation. <i>Biophysical Society, San Francisco CA.</i> (Poster)	2018
[5] Human Islet Amyloid Polypeptide: Identifying Early-Stage Aggregation Mechanisms through Molecular Simulation. <i>AIChE Annual Meeting, Minneapolis MN.</i> (Oral)	2017
[4] Amyloidogenic Proteins: Identifying Early-stage Aggregation Mechanisms. <i>Mind Bytes Symposium, University of Chicago</i> (Poster)	2017
[3] Early-Stage Aggregation of Human Islet Amyloid Polypeptide. <i>APS March Meeting, New Orleans LA.</i> (Oral)	2017
[2] Characterization of Self-associating and Complementary Polymers used to Control Fuel Mistig. <i>Summer Undergraduate Research Fellowship Seminar, Caltech</i> (Oral)	2012
[1] Design of a Program for Shear Induced Polymer Crystallization Control. <i>Summer Undergraduate Research Fellowship Seminar, Caltech</i> (Oral)	2011

Teaching	Instructor , 14:155:307 Computational Methods in ChE, Rutgers-NB	SP2024, SP2025, SP2026
	Co-Instructor , Grounds for Chemical Engineering, Rutgers-NB	SP2026
	Instructor , 14:155:309 ChE Thermodynamics II, Rutgers-NB	FA2023, FA2025
	Guest Lecturer , 16:155:605 Teaching in the Engineering Curriculum, Rutgers-NB	SP2025
	Guest Lecturer , 14:155:555 Advanced Materials in ChE, Rutgers-NB	SP2024
	Chicago Center for Teaching Fellow , UChicago	2018–2019
	Co-Instructor , MICCoM Enhanced Sampling for Molecular Simulations Tutorial	July 2017
	Teaching Assistant , Collegiate Scholars Program, Intro to Engineering Lab	Summer 2016
	Teaching Assistant , MENG 27300/32500: Polymer Physics & Eng., UChicago	Autumn 2015
	Dean's Tutor , Ch 21b: Physical Chemistry, Caltech	2014
Professional Activities	Teaching Assistant , Ch 3x: Experimental Methods in Solar Energy, Caltech	2013, 2014
	Guest Editor , <i>Entropy</i> , Special Issue: Molecular Modeling and Simulation	2026
	Book Reviewer , Pearson/Numerical Methods	2025

	Proposal Reviewer , Department of Energy (DOE) BES/CPIMS, National Science Foundation (NSF) CBET, NSF Industry-University Cooperative Research Centers (IUCRC), NSF Graduate Research Fellowships Program (GRFP)	2024–
	Independent Reviewer , ACS Macro. Letters, Macromolecules, Molecular Simulation, European Physical Journal E, Science Advances	2019–
	Session Chair , AIChE Annual Meeting (CoMSEF/1A, 8F), Foundations of Molecular Modeling and Simulation (FOMMS), EQUIFASE	2018–
Departmental & University Service	CBE Faculty Search Committee	2025–
	CBE ALChemE 3D Committee	2025–
	Founding Instructor , Rutgers Honors Engineering Experience (RHEX)	2024–
	CBE Graduate Admissions Committee	2024–
	ID3EA First Year Course , CBE Representative and Faculty Panelist	2024–
	CBE PhD Panel Series , Co-Developer	2024–
	CBE OXE Honor Society Faculty Advisor	2023–
	CBE Graduate Student Organization Faculty Advisor	2023–
	Rutgers CBE Thesis Committees: Lingjun Lu (Androulakis), Shivam Parashar (Neimark), Jinwoong Nam (Celik), Nicholas Corrente (Neimark), Haider Ejaz (Celik), Carlin Leung (Glasser), Austin Seamann (Khare/Chundawat), Yiwei Shao (Dutt), Val Rodrigues (Dignon)	
	External Thesis Committees: Aldo Vasquez (Ramirez-Hernandez, UT San Antonio Physics), Atul Thakur (Remsing, Rutgers CCB), Carlos Marquez Ibarra (Mayer, UT San Antonio Physics)	
Mentorship	Graduate Students (5) Mansi Gokani (PhD student at Rutgers-NB) Benjamin Borow (PhD student at Rutgers-NB) Kaelyn Chang (MS student at Rutgers-NB) Samiyah Siddiqui (MS student at Rutgers-NB) Chuting Deng (PhD student at University of Chicago → Postdoc at Northwestern University)	
	Undergraduates (5) Brianna Fea (UG student at Rutgers-NB, Aresty RA) Jean Chen (UG student at Rutgers-NB, Aresty RA) Julietta Straviou (UG student at Georgia Tech, visiting summer researcher) Gabriela Basel (UG student at University of Chicago → PhD student at Stanford) Drew Melchert (UG student at University of Chicago → PhD student at UCSB)	