

Contact/Bio	Engineering C-164 Rutgers University-New Brunswick	Email: <a href="mailto:ashley.guo@rutgers.edu">ashley.guo@rutgers.edu</a> Homepage: <a href="http://azguo.github.io">http://azguo.github.io</a>	Born: Norfolk, VA USA (US Citizen)
Appointments	<b>Rutgers, The State University of New Jersey</b> , New Brunswick NJ Assistant Professor, Department of Chemical and Biochemical Engineering		Sept 2023–
	<b>New York University</b> , New York NY Postdoctoral Associate, Center for Soft Matter Research, Advisor: Paul Chaikin		2020–2023
Education	<b>University of Chicago</b> , Chicago IL Ph.D., Molecular Engineering, Advisor: Juan de Pablo		2014–2020
	<b>California Institute of Technology</b> , Pasadena CA B.S., Chemical Engineering (Materials track), Advisor: Julie Kornfield		2010–2014
Fellowships, Leadership & Awards	<b>Faculty Excellence in Teaching and Advising Award</b> , Rutgers CBE <b>Distinguished Young Scholar</b> , University of Washington Chemical Engineering <b>William Rainey Harper Dissertation Fellow</b> , University of Chicago <b>Chicago Center for Teaching Fellow</b> , University of Chicago <b>Science Communication Fellow</b> , Museum of Science & Industry, Chicago IL <b>Arts, Culture, &amp; Science Initiative Graduate Fellow</b> , University of Chicago <b>Howard Hughes Medical Institute Teaching Fellow</b> , Caltech <b>Reed and Ruth Brantley Undergraduate Research Fellow</b> , Caltech		2024 2022 2018–2019 2018–2019 2015–2017 2015–2016 2014 2012
Publications * equal contribution	<p>[10] Wilken, S.*, <b>Guo, A.Z.*</b>, Levine, D., Chaikin, P.M., “Dynamical Approach to the Jamming Problem”, Phys. Rev. Lett., 131, 238202 (2023). [<a href="https://doi.org/10.1103/PhysRevLett.131.238202">doi:10.1103/PhysRevLett.131.238202</a>]</p> <p>[9] Fowler, W.C., Deng, C., Griffen, G.M., Teodoro, T., <b>Guo, A.Z.</b>, 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). [<a href="https://doi.org/10.1021/jacs.1c01241">doi:10.1021/jacs.1c01241</a>]</p> <p>[8] Sevgen, E., <b>Guo, A.Z.</b>, 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). [<a href="https://doi.org/10.1021/acs.jctc.9b00883">doi:10.1021/acs.jctc.9b00883</a>]</p> <p>[7] Colón, Y.J., <b>Guo, A.Z.</b>, Antony, L.B., Hoffmann, K.Q., de Pablo, J.J., “Free Energy of Metal Organic Framework Self-Assembly”, J. Chem. Phys., 150, 104502 (2019). [<a href="https://doi.org/10.1063/1.5063588">doi:10.1063/1.5063588</a>]</p> <p>[6] <b>Guo, A.Z.</b>, Lequieu, J., de Pablo J.J., “Extracting collective motions underlying nucleosome dynamics via the diffusion map”, J. Chem. Phys., 150, 054902 (2019). [<a href="https://doi.org/10.1063/1.5063851">doi:10.1063/1.5063851</a>]</p> <p>[5] <b>Guo, A.Z.</b>, Fluitt, A.M., de Pablo, J.J., “Early-stage Human Islet Amyloid Polypeptide Aggregation: Mechanisms Behind Dimer Formation”, J. Chem. Phys., 149, 025101 (2018). [<a href="https://doi.org/10.1063/1.5033458">doi:10.1063/1.5033458</a>]</p> <p>[4] <b>Guo, A.Z.*</b>, 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). [<a href="https://doi.org/10.1063/1.5020733">doi:10.1063/1.5020733</a>]</p> <p>[3] Sidky, H., Colón, Y.J., Helfferich, J., Sikora, B.J., Bezik, C., Chu, W., Giberti, F., <b>Guo, A.Z.</b>, 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). [<a href="https://doi.org/10.1063/1.5008853">doi:10.1063/1.5008853</a>]</p> <p>[2] Sadati, M., Zhou, Y., Melchert, D., <b>Guo, A.</b>, 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](https://doi.org/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](https://doi.org/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](https://doi.org/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*.

#### 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. *AIChE Annual Meeting, San Diego CA* (Oral) 2024  
 [21] A Data- and Information-Driven Approach for Computational Soft Materials Design. *5th Molecular Simulations Workshop, NJIT* (Poster) 2024  
 [20] A Data- and Information-Driven Approach for Computational Soft Materials Design. *FOMMS, Snowbird UT* (Poster) 2024  
 [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. *AIChE Annual Meeting, Phoenix AZ* (Oral) 2022  
 [17] An Information-Driven Approach for Controlling Emergent Order in Soft Materials. *AIChE Annual Meeting, Phoenix AZ* (Poster) 2022  
 [16] An Information-driven Approach to Quantifying and Controlling 2022

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

	<b>Independent Reviewer</b> , ACS Macro. Letters, Macromolecules, Molecular Simulation, European Physical Journal E, Science Advances	2019–
	<b>Session Chair</b> , AIChE Annual Meeting (CoMSEF/1A, 8F), Foundations of Molecular Modeling and Simulation (FOMMS), EQUIFASE	2018–
Departmental & University Service	<b>CBE Faculty Search Committee</b>	2025–
	<b>Founding Instructor</b> , Rutgers Honors Engineering Experience	2024–
	<b>CBE Graduate Admissions Committee</b>	2024–
	<b>ID3EA First Year Course</b> , CBE Representative and Faculty Panelist	2024–
	<b>CBE PhD Panel Series</b> , Co-Developer	2024–
	<b>CBE OXE Honor Society Faculty Advisor</b>	2023–
	<b>CBE Graduate Student Organization Faculty Advisor</b>	2023–
	<b>Rutgers CBE Thesis Committees:</b> 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)	
	<b>External Thesis Committees:</b> Aldo Vasquez (Ramirez-Hernandez, UT San Antonio Physics), Atul Thakur (Remsing, Rutgers CCB), Carlos Marquez Ibarra (Mayer, UT San Antonio Physics)	
Mentorship	<b>Graduate Students (5)</b> 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)	
	<b>Undergraduates (5)</b> Brianna Fea (UG student at Rutgers-NB, Aresty RA) Jean Chen (UG student at Rutgers-NB, Aresty RA) Julieta 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)	