Ashley Z. Guo 18 Jan 2026

Contact/Bio

Engineering C-164
Rutgers University-New Brunswick

Email: ashley.guo@rutgers.edu
Homepage: http://azguo.github.io

Born: Norfolk, VA USA
(US Citizen)

Appointments

Rutgers, The State University of New Jersey, New Brunswick NJ — Sept 2023–
Assistant Professor, Department of Chemical and Biochemical Engineering

New York University, New York NY — 2020–2023
Postdoctoral Associate, Center for Soft Matter Research, Advisor: Paul Chaikin

Education

University of Chicago, Chicago IL — 2014–2020
Ph.D., Molecular Engineering, Advisor: Juan de Pablo

California Institute of Technology, Pasadena CA — 2010–2014
B.S., Chemical Engineering (Materials track), Advisor: Julie Kornfield

Fellowships, Leadership & Awards

Faculty Excellence in Teaching and Advising Award, Rutgers CBE — 2024
Distinguished Young Scholar, University of Washington Chemical Engineering — 2022
William Rainey Harper Dissertation Fellow, University of Chicago — 2018–2019
Chicago Center for Teaching Fellow, University of Chicago — 2018–2019
Science Communication Fellow, Museum of Science & Industry, Chicago IL — 2015–2017
Arts, Culture, & Science Initiative Graduate Fellow, University of Chicago — 2015–2016
Howard Hughes Medical Institute Teaching Fellow, Caltech — 2014
Reed and Ruth Brantley Undergraduate Research Fellow, Caltech — 2012

Publications

* equal contribution

[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]

[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]

[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]

[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]

[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]

[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]

[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]

[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]

[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

(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.*

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 2024
Separation Via Data Compression. *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 2022
Emergent Order. *AIChE Annual Meeting, Phoenix AZ* (Oral)

[17] An Information-Driven Approach for Controlling Emergent Order in 2022
Soft Materials. *AIChE Annual Meeting, Phoenix AZ* (Poster)

[16] An Information-driven Approach to Quantifying and Controlling 2022

Emergent Order. *Univ. of Washington Distinguished Young Scholars Seminar* (Oral)

[15] Higher Dimensional Biased Random Organization 2022
APS March Meeting, Chicago IL (Oral)

[14] Characterizing phase transitions in 2D Repulsive Random Organization 2021
APS March Meeting, Virtual Talk (Oral)

[13] Identifying Trimerization Mechanisms of Human Islet Amyloid Polypeptide 2019
through Molecular Simulation. *APS March Meeting, Boston MA.* (Oral)

[12] Nonlinear Manifold Learning of Nucleosome Dynamics from Molecular Simulation 2018
AIChE Annual Meeting, Pittsburgh PA. (Oral)

[11] Human Islet Amyloid Polypeptide: Identifying Early-Stage Aggregation 2018
Mechanisms through Molecular Simulation. *EQUIFASE 2018, Córdoba, Argentina.* (Oral)

[10] Understanding Nucleosome Dynamics using Diffusion Maps 2018
Frontiers of Molecular Engineering, Chicago IL (Poster, Best Poster Award)

[9] Understanding Nucleosome Dynamics using Diffusion Maps 2018
Mind Bytes Symposium, University of Chicago Research Computing Center (Poster)

[8] Human Islet Amyloid Polypeptide: Identifying Early-Stage Aggregation Mechanisms 2018
through Molecular Simulation. *Mind Bytes Symposium, University of Chicago* (Poster)

[7] Extracting collective motions underlying nucleosome dynamics via nonlinear 2018
manifold learning. *APS March Meeting, Los Angeles CA.* (Oral)

[6] Human Islet Amyloid Polypeptide: Identifying Early-Stage Aggregation Mechanisms 2018
through Molecular Simulation. *Biophysical Society, San Francisco CA.* (Poster)

[5] Human Islet Amyloid Polypeptide: Identifying Early-Stage Aggregation Mechanisms 2017
through Molecular Simulation. *AIChE Annual Meeting, Minneapolis MN.* (Oral)

[4] Amyloidogenic Proteins: Identifying Early-stage Aggregation Mechanisms. 2017
Mind Bytes Symposium, University of Chicago (Poster)

[3] Early-Stage Aggregation of Human Islet Amyloid Polypeptide. 2017
APS March Meeting, New Orleans LA. (Oral)

[2] Characterization of Self-associating and Complementary Polymers used to Control 2012
Fuel Misting. *Summer Undergraduate Research Fellowship Seminar, Caltech* (Oral)

[1] Design of a Program for Shear Induced Polymer Crystallization Control. 2011
Summer Undergraduate Research Fellowship Seminar, Caltech (Oral)

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
Teaching Assistant, Ch 3x: Experimental Methods in Solar Energy, Caltech 2013, 2014

Professional Activities

Guest Editor, *Entropy*, 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 2019–

Simulation, European Physical Journal E, Science Advances
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–
Founding Instructor, Rutgers Honors Engineering Experience 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)