Ashley Z. Guo 18 Jan 2026

Contact/Bio

Engineering C-164
Rutgers University-New Brunswick

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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 Fellowship, University of Chicago — 2018–2019
Chicago Center for Teaching Fellow, University of Chicago — 2018–2019
Society of Women Engineers, Co-founder & Treasurer, University of Chicago — 2017–2018
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
American Institute of Chemical Engineers – Chapter President, Caltech — 2012–2013
Reed and Ruth Brantley Undergraduate Research Fellow, Caltech — 2012

Publications

(* denotes 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 Emergent Order. *Univ. of Washington Distinguished Young Scholars Seminar* (Oral) 2022

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

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

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

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

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

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

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

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

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

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

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

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

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

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

[1] Design of a Program for Shear Induced Polymer Crystallization Control. *Summer Undergraduate Research Fellowship Seminar, Caltech* (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
Teaching Assistant, Ch 3x: Experimental Methods in Solar Energy, Caltech 2013, 2014
(Supported by Howard Hughes Medical Institute in 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 2024–

(IUCRC), NSF Graduate Research Fellowships Program (GRFP)

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–

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–

OXE Honor Society Faculty Advisor, Rutgers-NB — 2023–

CBE Graduate Student Organization Faculty Advisor, Rutgers-NB — 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)