

Kateri H. DuBay
Associate Professor of Chemistry
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APPOINTMENTS

- | | |
|-------------|---|
| Current | Associate Professor of Chemistry, University of Virginia, 2023
Assistant Professor of Chemistry, University of Virginia, 2014-2023 |
| 2010 - 2013 | Postdoctoral Research Scientist, Columbia University, NY
Advisors: David Reichman and Richard Friesner |
| 2009 - 2010 | Postdoctoral Scholar, University of California, Berkeley
Advisors: Phillip Geissler and Dirk Trauner |

EDUCATION

University of California, Berkeley

Ph.D. in Chemistry, December 2009

Advisor: Phillip Geissler

University of Cambridge, UK

M.Phil. in Chemistry, March 2004

Advisors: Sir Christopher Dobson and Michele Vendruscolo

Georgetown University, DC

B.S. in Biochemistry, *summa cum laude*, May 2002

Honors Thesis Advisor: Paul Roepe

SELECTED HONORS AND AWARDS

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|------|--|
| 2022 | American Chemical Society COMP Division OpenEye Outstanding Junior Faculty Award |
| 2020 | Cottrell Scholar Award |
| 2020 | UVA Research Award |
| 2020 | UVA College Fellow – selected to teach in the New College Curriculum |
| 2019 | NSF CAREER Award |
| 2019 | Junior Faculty Poster Prize, Berkeley Statistical Mechanics Meeting |
| 2018 | Alumni Board of Trustees Teaching Award, UVA |
| 2017 | Cory Family Teaching Award, College of Arts and Sciences, UVA |
| 2016 | Mead Honored Faculty, UVA |
| 2004 | NSF Graduate Research Fellowship, UC Berkeley |
| 2003 | Berkeley Fellowship, UC Berkeley |
| 2002 | Gates Cambridge Scholar, University of Cambridge |

RESEARCH ARTICLES Total Citation Count: 1982; h-index: 14 (Google Scholar, 8/25/2023)

25. G. R. Bowman, S. J. Cox, C. Dellago, **K. H. DuBay**, J. D. Eaves, D. A. Fletcher, L. B. Frechette, M. Grünwald, K. Klymko, J. Ku, A. Omar, E. Rabani, D. R. Reichman, J. R. Rogers, A. M. Rosnik, G. M. Rotskoff, A. R. Schneider, N. Schwierz, D. A. Sivak, S. Vaikuntanathan, S. Whitelam, and A. Widmer-Cooper. Remembering the work of Phillip L. Geissler: A coda to his scientific trajectory. *Annu Rev Phys Chem* (2023) 74, 1-27. DOI: [10.1146/annurev-physchem-101422-030127](https://doi.org/10.1146/annurev-physchem-101422-030127)
24. N. Nguyen*, R. Hamblin*, **K. H. DuBay**. Emergent sequence biasing in step-growth copolymerization: influence of non-bonded interactions and comonomer reactivities. *J Phys Chem B* (2022) 126, 6585-6597. DOI: [10.1021/acs.jpcc.2c04092](https://doi.org/10.1021/acs.jpcc.2c04092) *These authors contributed equally.
◆ Selected for [Cover Feature](#)
23. Q. Jia, B. J. Venton and **K. H. DuBay**. Structure and Dynamics of Adsorbed Dopamine on Solvated Carbon Nanotubes and in a CNT Groove. *Molecules* (2022) 27, 3768. DOI:[10.3390/molecules27123768](https://doi.org/10.3390/molecules27123768)
◆ Selected for [Cover Feature](#)
22. Q. Jia, C Yang, B. J. Venton and **K. H. DuBay**. Atomistic simulations of dopamine diffusion dynamics on a pristine graphene surface. *ChemPhysChem* (2022) 23, e202100783. DOI:[10.1002/cphc.202100783](https://doi.org/10.1002/cphc.202100783)
21. R. L. Hamblin, N. Q. Nguyen and **K. H. DuBay**. Selective solvent conditions influence sequence development and supramolecular assembly in step-growth copolymerization. *Soft Matter* (2022) 18, 943-955. DOI:[10.1039/D1SM01571K](https://doi.org/10.1039/D1SM01571K)
◆ Selected for [Cover Feature](#)
20. Z. Zhang and **K. H. DuBay**. The Sequence of a Step-Growth Copolymer Can Be Influenced by Its Own Persistence Length. *J Phys Chem B* (2021) 125, 3426-37. DOI:[10.1021/acs.jpcc.1c00873](https://doi.org/10.1021/acs.jpcc.1c00873)
19. D. A. Nyenhuis, T. D. Nilaweera, J. K. Niblo, N. Q. Nguyen, **K. H. DuBay**, and D. S. Cafiso. Evidence for the Supramolecular Organization of a Bacterial Outer-Membrane Protein from In-Vivo Pulse EPR Spectroscopy. *J Am Chem Soc* (2020) 142, 10714-22. DOI:[10.1021/jacs.0c01754](https://doi.org/10.1021/jacs.0c01754)
18. Z. Zhang and **K. H. DuBay**. Modeling the influence of emergent and self-limiting phase separations among nascent oligomers on polymer sequences formed during irreversible step-growth copolymerizations. *Macromolecules* (2019) 52:15, 5480-5490. DOI:[10.1021/acs.macromol.9b00266](https://doi.org/10.1021/acs.macromol.9b00266)
17. S. N. Merz, E. Hoover, S. A. Egorov, **K. H. DuBay***, and D. L. Green*. Predicting the Effect of Chain-Length Mismatch on Phase Separation in Noble Metal Nanoparticle Monolayers with Chemically Mismatched Ligands. *Soft Matter* (2019) 15, 4498. DOI:[10.1039/C9SM00264B](https://doi.org/10.1039/C9SM00264B) *Co-corresponding authors.
16. S. N. Merz, Z. J. Farrell, J. Pearring, E. Hoover, M. Kester, S. A. Egorov, D. L. Green*, and **K. H. DuBay***. Computational and Experimental Investigations of Janus-like Monolayers on Ultrasmall Noble Metal Nanoparticles. *ACS Nano*. (2018) 12, 11031-40. DOI:[10.1021/acs.nano.8b05188](https://doi.org/10.1021/acs.nano.8b05188) *Co-corresponding authors.
15. **K. H. DuBay**, K. Iwan, L. Osorio-Planes, P. L. Geissler, M. Groll, D. Trauner, and J. Broichhagen. A predictive approach for the optical control of carbonic anhydrase II activity. *ACS Chem Biol*. (2018) 13, 793-800. DOI:[10.1021/acscchembio.7b00862](https://doi.org/10.1021/acscchembio.7b00862)
14. X. Zhu, S. R. Bheemireddy, S. V. Sambasivarao, P. W. Rose, R. T. Guzman, A. G. Waltner, **K. H. DuBay***, and K. N. Plunkett*. Construction of Donor-Acceptor Polymers via Cyclopentannulation of Poly(arylene ethynylene)s. *Macromolecules* (2016) 49, 127-133. DOI:[10.1021/acs.macromol.5b02061](https://doi.org/10.1021/acs.macromol.5b02061) *Co-corresponding authors.

◆ *Highlighted in Synfacts, (2016) 12, 0250.*

13. **K. H. DuBay**, G. Bowman, and P. L. Geissler. Fluctuations within folded proteins: Implications for thermodynamic and allosteric regulation. *Acc Chem Res* (2015) 48, 1098-105. DOI:[10.1021/ar500351b](https://doi.org/10.1021/ar500351b)

Prior to UVA

12. A. L. Weisman, **K. H. DuBay**, K. A. Willets, and R. A. Friesner. A First-Principles Polarized Raman Method for Determining Whether a Uniform Region of a Sample is Crystalline or Isotropic. *J Chem Phys* (2014) 141, 224702. DOI:[10.1063/1.4903308](https://doi.org/10.1063/1.4903308)
11. E. J. Dell, B. Capozzi, **K. H. DuBay**, T. C. Berkelbach, J. R. Moreno, D. R. Reichman, L. Venkataraman, and L. M. Campos. Impact of Molecular Symmetry on Single-Molecule Conductance. *J Am Chem Soc.* (2013) 135, 11724-7. DOI:[10.1021/ja4055367](https://doi.org/10.1021/ja4055367)
10. M. C. Traub, **K. H. DuBay**, S. E. Ingle, X. Zhu, K. N. Plunkett, D. R. Reichman, and D. A. Vanden Bout. Chromophore-Controlled Self-Assembly of Highly Ordered Polymer Nanostructures. *J Phys Chem Lett* (2013) 4:15, 2520-4. DOI:[10.1021/jz401114y](https://doi.org/10.1021/jz401114y)
9. **K. H. DuBay**, M. L. Hall, T. F. Hughes, C. Wu, D. R. Reichman, and R. A. Friesner. Accurate Force Field Development for Modeling Conjugated Polymers. *J Chem Theory Comput* (2012) 8, 4556-69. DOI:[10.1021/ct300175w](https://doi.org/10.1021/ct300175w)
8. J. C. Heckel, A. L. Weisman, S. T. Schneebeli, M. L. Hall, L. J. Sherry, S. M. Stranahan, **K. H. DuBay**, R. A. Friesner, and K. A. Willets. Polarized Raman Spectroscopy of Oligothiophene Crystals To Determine Unit Cell Orientation. *J Phys Chem A* (2012) 116, 6804-16. DOI:[10.1021/jp304192v](https://doi.org/10.1021/jp304192v)
7. G. Bounos, S. Ghosh, A. K. Lee, K. N. Plunkett, **K. H. DuBay**, J. C. Bolinger, R. Zhang, R. A. Friesner, C. Nuckolls, D. R. Reichman, and P. F. Barbara. Controlling Chain Conformation in Conjugated Polymers Using Defect Inclusion Strategies. *J Am Chem Soc* (2011) 133:26, 10155-60. DOI:[10.1021/ja2006687](https://doi.org/10.1021/ja2006687)
6. **K. H. DuBay**, J. P. Bothma, and P. L. Geissler. Long-Range Intra-Protein Communication Can Be Transmitted by Correlated Side-Chain Fluctuations Alone. *PLoS Comput Biol* (2011) 7:9, e1002168. DOI:[10.1371/journal.pcbi.1002168](https://doi.org/10.1371/journal.pcbi.1002168)
5. **K. H. DuBay** and P. L. Geissler. Calculation of Proteins' Total Side-Chain Torsional Entropy and Its Influence on Protein-Ligand Interactions. *J Mol Biol* (2009) 391, 484-97. DOI:[10.1016/j.jmb.2009.05.068](https://doi.org/10.1016/j.jmb.2009.05.068)
4. A. P. Pawar*, **K. F. DuBay***, J. Zurdo, F. Chiti, M. Vendruscolo, and C. M. Dobson. Prediction of "Aggregation-prone" and "Aggregation-susceptible" Regions in Proteins Associated with Neurodegenerative Diseases. *J Mol Biol* (2005) 350, 379-92. DOI:[10.1016/j.jmb.2005.04.016](https://doi.org/10.1016/j.jmb.2005.04.016)
*These authors contributed equally.
◆ *Recognized as one of the top 10 downloaded papers from JMB in 2005.*
3. **K. F. DuBay**, A. P. Pawar, F. Chiti, J. Zurdo, C. M. Dobson, and M. Vendruscolo. Prediction of the Absolute Aggregation Rates of Amyloidogenic Polypeptide Chains. *J Mol Biol* (2004) 341, 1317-26. DOI:[10.1016/j.jmb.2004.06.043](https://doi.org/10.1016/j.jmb.2004.06.043)
2. A. Leed*, **K. DuBay***, L. M. B. Ursos, D. Sears, A. C. de Dios, and P. D. Roepe. Solution Structures of Antimalarial Drug-Heme Complexes. *Biochemistry* (2002) 41, 10245-55. DOI:[10.1021/bi020195i](https://doi.org/10.1021/bi020195i)
*These authors contributed equally.

1. L. M. B. Ursos, **K. F. DuBay**, and P. D. Roepe. Antimalarial Drugs Influence the pH Dependent Solubility of Heme via Apparent Nucleation Phenomena. *Mol Biochem Parasitol* (2001) 112, 11-17. DOI:[10.1016/S0166-6851\(00\)00342-X](https://doi.org/10.1016/S0166-6851(00)00342-X)

PATENTS

4. European Patent No. 2261670. C. M. Dobson, F. Chiti, J. Zurdo, **K. H. DuBay**, and M. Vendruscolo. Method and Apparatus for Assessing Polypeptide Aggregation. Issued: August 20, 2014.
3. US Patent No. 8155888. C. M. Dobson, F. Chiti, J. Zurdo, **K. H. DuBay**, and M. Vendruscolo. Method and Apparatus for Assessing Polypeptide Aggregation. Issued: April 10, 2012.
2. European Patent No. 1680681. C. M. Dobson, F. Chiti, J. Zurdo, **K. H. DuBay**, and M. Vendruscolo. Method and Apparatus for Assessing Polypeptide Aggregation. Issued: November 2, 2011.
1. US Patent No. 7698070. C. M. Dobson, F. Chiti, J. Zurdo, **K. H. DuBay**, and M. Vendruscolo. Method and Apparatus for Assessing Polypeptide Aggregation. Issued: April 13, 2010.

Claims for patents 1,2, and 4 are based on Ref. 4 above. Claims for patent 3 are based on Ref. 3 above.

TEACHING EXPERIENCE

CHEM 5220 — Advanced Physical Chemistry II: Statistical Mechanics
Fall 2015, Fall 2016, Fall 2017, Fall 2018 & Fall 2022, The University of Virginia

CHEM 7020 — Research Seminar II: Research Innovation, Entrepreneurship, and Ethics
Spring 2023, The University of Virginia

EGMT 1510 — Engaging Aesthetics: In Praise of Entropy
Fall 2020, Spring 2021, Fall 2021 & Spring 2022, The University of Virginia

CHEM 2820 — Principles of Chemical Thermodynamics and Kinetics
Spring 2015, Spring 2016, Spring 2017 & Spring 2019, The University of Virginia

Professional Teaching Development

- UVA Course Design Institute, a week-long course with the Center for Teaching Excellence, 2015
- Cottrell Scholars Collaborative New Faculty Workshop weekend for chemistry faculty, 2015
- Center for Teaching Excellence's year-long faculty development Ignite Program, 2015-2016
- Consultation with Learning Design & Technology regarding course website design
- Consultation with the CTE on best DEI practices when covering a sensitive topic

PROFESSIONAL SERVICE

Department

- Majors Advising, Chemistry Department, 2015 - present
- Transfer Student Advisor, 2020 - present (approx. 40 advisees)
- Chemistry Dept Executive Committee, voted in as the Assistant Professor Member, 2016-2017 & 2021-2022
- Undergraduate Studies Committee Member, 2020 - present
- Poster Judge at the 3rd Year Graduate Student Poster session, 2022
- Graduate Student First Year Course Advising for Physical Chemistry, 2021 - present
- UVA New Faces in Chemistry – A Future Faculty Workshop, panelist for Research Statement session, 2021

- National Chemistry Week Speaker for the ACS Student Chapter at UVA: *How it began, circa 2002: I can tutor anything except thermo. How it's going, circa 2020: I only teach thermo, 2020*
- Member of Multiple Chemistry Candidacy, MA/MS, and PhD Thesis Committees, UVA, 2015 - present
- Chemistry Building Renovations, Theory Liaison, 2016-2019
- Seminar Committee, Chemistry Department, 2014-2019
- Graduate Admissions and Recruitment Committee, Chemistry Department, UVA, 2014-2018
 - Physical Chemistry Subcommittee Chair, 2017-2018
- Chemistry Department Peer Evaluation Committee on Teaching and Service, 2017

University

- Chair of the College of A&S Ad Hoc Committee on SCHEV Guaranteed Admission Agreement, 2023
- UVA Engagements Experience Speaker on Empirical Learning – served as the keynote speaker at one of four required lectures for all first year Engagement Students, 2023
- UVA NSF CAREER Program Workshop Panelist, 2021
- UVA Admitted Students Science & Math Panelist, 2021
- UVA College Fellows Faculty Shop Talk 2020: *Into the Unknown: Self-Protective and Self-Limiting Habits in Learning*
- Graduate Student Teaching Awards Selection Committee, UVA, 2019
- Undergraduate Fellowship Nomination and Practice Interviews with UVA's Office of Citizen Scholar Development, 2018-2022
- New College Curriculum Assessment Committee, College of Arts & Sciences, UVA, 2017-2019
- Served as a summer mentor for Leadership Alliance student, Marcus Jordan, who participated as part of the Medical School's SRIP program, Summer 2017
- Keynote Speaker at the UVA Undergraduate Research Network Meeting on Women in Research, 2015
- Member of Candidacy and PhD Thesis committees, UVA: Chemical Engineering, Biomedical Engineering, 2014 - present
- Provided numerous letters of recommendation to both undergraduate and graduate students, 2014 - present

National Professional Service and Community Engagement

- Session Chair at the Berkeley Statistical Mechanics Meeting, 2023
- Coordinated Chemistry and Biology Dept donations of PPE to health care providers during the first wave of Covid-19, 2020
- Poster Judge at the Berkeley Statistical Mechanics Meeting, 2019
- Poster Judge at the Materials Research Society National Meeting, 2018
- Session Chair at the Berkeley Statistical Mechanics Meeting, 2017
- Session Chair at the Virginia Soft Matter Workshop, 2015
- Peer Reviewer for Journal Articles in: *Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Macromolecules, Physical Chemistry Chemical Physics, PLoS One, Computer Physics Communications, Nanoscale Advances, Macromolecular Theory and Simulations, Biomacromolecules*
- Grant Reviewer for ACS PRF, NSF (*ad hoc and panelist*), Research Corporation for Science Advancement
- American Chemical Society, Member, ID # 31649925
 - *Current Technical Divisions:* Computers in Chemistry & Polymeric Materials Science & Engineering

RESEARCH ADVISING

Postdoctoral Advisees

- Dr. Jessica Niblo, 2022-present
- Dr. Steven Merz, 2018-2020 (*Current: Data Scientist at Highmark Health*)
- Dr. Venkata Sambasivarao Somiseti, 2014-2015

Graduate PhD Students

Current:

- Jacob Swartley, Chemistry, 2017-present
- Nhu Nguyen, Chemistry, 2018-present
- Ryan Hamblin, Chemistry, 2019-present
 - *High Pass on Candidacy Exam, 2021*
 - *NSF GRFP Honorable Mention, 2021*
- Wenxin Xu, Chemistry, 2021-present
- Zachary LaFaver, 2022-present

Past:

- Jessica Niblo, PhD in Chemistry, 2022 (*Current: Postdoc with UVA Engagements Program*)
 - *Distinguished Graduate Teaching Award for STEM Fields, 2018*
 - *Outstanding Graduate Teaching Assistant Award, 2018*
- Zhongmin Zhang, PhD in Chemistry, 2020 (*Current: Postdoc with Zhiyue Lu at UNC-CH*)
- Qizhang Jia, PhD in Chemistry, 2020 (*Current: Google Software Engineer*)
- Spencer Lovrinic, MA in Chemistry, 2021

Graduate Students from UVA's Terminal MA Program in Chemistry

Kelly Carr, MA Chemistry, 2017 (*Current: Data Operations Specialist at Center for Diabetes Technology, UVA*)
 Zhongmin Zhang, MA Chemistry, 2016 (*stayed on for a doctorate, earned PhD in 2020*)
 Qishen Huang, MA Chemistry, 2016, (*PhD in Civil and Environmental Engineering at VA Tech, 2021*)

Undergraduate Students

Casey Zhang, 2022-present
 Michelle Lwin, 2022-present
 Wamia Said, 2022-2023
 David Gepitulan, 2022
 Pablo Fernandez, 2020-2022 (*PhD student at UNC-CH*)
 Tatiana Kennedy, 2021-2022 (*Current: Cheminformatics Research Associate at Nurix Therapeutics*)
Lester Andrews Undergraduate Summer Research Scholarship
 Dade Carroll, Summer 2021
 Zagros Asadi, Summer 2021
 Akshat Zalte (IIT Bombay), Summer 2021
 Niraja Patankar (IIT Bombay), Summer 2021
 Lauryn Power, 2019-2021
 Austin Cheng, 2018-2021 (*PhD student at U Toronto*)
 Distinguished Majors Thesis: *Dynamic self-assembly of a colloidomer polyampholyte under oscillating pH*
Lester Andrews Undergraduate Summer Research Scholarship
 Xuanye (Claire) Zhu, 2017-2018
 Cory Kim, 2018
 Amy Wang, 2018
 Marcus Jordan (UMBC Chemistry, Leadership Alliance research student), Summer 2017
 Adam Antoszewski, 2015-2016 (*PhD in Chemistry at U Chicago, 2022*)
 Artemie Jurgenson, 2014-2016
 Thesis: *Modeling Metastable Nucleation Under Shear Using the Two-Dimensional Ising Model.*

RESEARCH PRESENTATIONS

PI Presentations and Seminars

44. Berkeley Statistical Mechanics Meeting – Phillip Geissler Memorial Symposium, Berkeley, CA, January 2023
43. Informal Statistical Physics Seminar, University of Maryland, MD, November 2022
42. Chemistry Department Seminar, Duke University, Durham, NC, September 2022
41. Chemistry Department Seminar, University of Virginia, VA, September 2022
40. Condensed Phase Dynamics, TSRC, Telluride, CO, July 2022
39. Chemistry Department, University of Chicago, IL, March 2022

38. Chemical Physics Seminar, Caltech, CA, March 2022
37. Physical Chemistry Seminar, UC Berkeley, CA, March 2022
36. Chemistry Department Seminar, New York University, NY, February 2022
35. Chemistry Department Colloquium, Columbia University, NY (*presented virtually*), January 2022
34. Laufer Center and Chemistry Joint Seminar, Stony Brook University, NY (*presented virtually*), December 2021
33. Chemistry Dept. Seminar, Trinity College, CT (*presented virtually*), October 2021
32. Theoretical Chemistry Seminar, Dept. of Chemistry, Stanford University, CA (*presented virtually*), May 2021
31. Physical Chemistry Seminar, Dept. of Chemistry, UNC – Chapel Hill, NC (*presented virtually*), October 2020
30. Research Webinar, Department of Chemistry and Biochemistry, U. of Wisconsin - Eau Claire, October 2020
29. Condensed Phase Dynamics, TSRC, Telluride, CO (*presented virtually*), July 2020
28. Cottrell Scholar Conference, Tucson, AZ (*presented virtually*), July 2020
27. *Gubbins Seminar, North Carolina State University, Raleigh, NC, April 2020 – canceled due to Covid-19*
26. Chemistry Seminar, Georgetown University, Washington, DC, February 2020
25. Berkeley Statistical Mechanics Meeting, UC Berkeley, CA, January 2020
24. nanoMedicine Symposium, Virginia Commonwealth U., Richmond, VA, November 2019
23. Physical Chemistry Seminar, University of Washington, Seattle, WA, October 2019
22. Biophysics & Soft Matter Seminar, Simon Fraser U, Vancouver, BC, October 2019
21. Physical Chemistry Seminar, University of Pennsylvania, Philadelphia, PA, October 2019
20. Squishy Materials Seminar, University of Virginia, Charlottesville, VA, September 2019
19. Dept of Chemistry, Physics and Geology Seminar, Winthrop Univ., Rock Hill, SC, September 2019
18. Virginia Soft Matter Workshop, University of Virginia, Charlottesville, VA, September 2019
17. Nanoscale Science Program Seminar, UNC Charlotte, Charlotte, NC, March 2019
16. Contributed Talk, Materials Research Society Fall Meeting, Boston, MA, November 2018
15. Chemistry Department Seminar, Skidmore College, Saratoga Springs, NY, November 2017
14. Seminar, Oak Ridge National Lab, Oak Ridge, TN, October 2017
13. Physical Chemistry Seminar, Columbia University, NY, March 2013
12. Chemistry Department Seminar, University of Miami, FL, February 2013
11. Chemistry Department Seminar, Drexel University, PA February 2013
10. Chemistry Department Seminar, University of North Carolina, Chapel Hill, NC, February 2013
9. Chemistry Department Seminar, University of Virginia, February 2013
8. Chemistry Department Colloquium, University of Georgia, Athens, GA, January 2013
7. Chemistry and Biochemistry Department Seminar, University of South Carolina, Columbia, SC, January 2013
6. Chemical Engineering and Materials Science Department Seminar, UC Davis, CA, January 2013
5. Physical-Theoretical Chemistry Seminar, University of Southern California, CA, January 2013
4. Chemistry Department Special Seminar, University of Chicago, IL, January 2013
3. Chemistry Department Seminar, North Carolina State University, Raleigh, NC, December 2012
2. Contributed Talk, Biophysical Society Annual Meeting, Long Beach, CA, February 2008
1. Contributed Talk, Biophysical Society Annual Meeting, Baltimore, MD, March 2007

Selected PI Poster Presentations

14. OpenEye Outstanding Junior Faculty Award Poster, ACS Fall Meeting, Chicago, August 2022
13. Polymer Physics Gordon Research Conference, Mt. Holyoke College, MA, July 2022
12. Soft Condensed Matter Physics Gordon Research Conference, Colby-Sawyer College, NH, August 2019
11. Self-Assembly and Supramolecular Chemistry Gordon Research Conference, Les Diablerets, Switzerland, May 2019
10. Berkeley Statistical Mechanics Meeting, Berkeley, CA, January 2019 ***Junior Faculty Poster Prize Winner**
9. Commonwealth Conference on National Defense and Intelligence Poster, Charlottesville, VA, June 2017

8. NSF Workshop on Complex Systems Poster Session, Arlington, VA, May 2017
7. Frontiers in Polymer Science, Seville, Spain, May 2017
6. Mini Stat Mech Meeting, Berkeley, CA, January 2014
5. Mini Stat Mech Meeting, Berkeley, CA, January 2012
4. Electronic Processes in Organic Materials Gordon Research Conference, Lucca, Italy, June 2012
3. Mini Stat Mech Meeting, Berkeley, CA, January 2011
2. Protein Folding Dynamics Gordon Research Conference, Ventura, CA, January 2010
1. Proteins Gordon Research Conference, Holderness, NH, June 2007

DuBay Group and Collaborator Presentations (*bold indicates the presenter; DuBay Group members are underlined*)

31. **Ryan L. Hamblin**, Zhongmin Zhang, and Kateri H. DuBay. Nematic ordering of nascent oligomers induces collective sequence development in step-growth copolymerization. *Berkeley Statistical Mechanics Meeting*, Berkeley, CA, January 2023 (*poster*).
30. **Jessica K. Niblo**, Jacob R. Swartley, Zhongmin Zhang, and Kateri H. DuBay. Modifying self-assembly of 2D viral capsid-like structures in a variable energy landscape. *Berkeley Statistical Mechanics Meeting*, Berkeley, CA, January 2023 (*poster*).
29. **Nhu Q. Nguyen**, Ryan L. Hamblin, and Kateri H. DuBay. Combined effect of non-bonded interactions and comonomer reactivities results in sequence biasing during step-growth copolymerization. *Berkeley Statistical Mechanics Meeting*, Berkeley, CA, January 2023 (*poster*).
28. **Nhu Q. Nguyen**, Ryan L. Hamblin, and Kateri H. DuBay. Sequence biasing in step-growth copolymerization: Combined effects of non-bonded interactions and relative activation energies. *ACS Fall National Meeting*, Chicago, IL, August 2022 (*poster*).
27. **Ryan L. Hamblin**, Nhu Q. Nguyen, and Kateri H. DuBay. Selective solvation in step-growth copolymerization drives emergent self-assembly and alters sequence development. *Systems Chemistry GRC*, Newry, ME, June 2022 (*poster*).
26. **Jessica K. Niblo**, Jacob R. Swartley, Zhongmin Zhang, and Kateri H. DuBay. Self-Assembly of 2D Viral Capsid-like Structures in a Variable Energy Landscape. *Systems Chemistry GRC*, Newry, ME, June 2022 (*poster*).
25. **Ryan L. Hamblin**, Nhu Q. Nguyen, and Kateri H. DuBay. Asymmetric monomer affinity in step-growth copolymerization: Self-assembly and sequence effects. *ACS Spring National Meeting*, San Diego, CA, March, 2022 (*virtual poster*).
24. **Jessica K. Niblo**, Jacob R. Swartley, Zhongmin Zhang and Kateri H. DuBay. Modifying self-assembly of 2D viral capsid-like structures via inter-particle potential variation. *ACS Fall National Meeting*, Atlanta, GA, August 2021 (*virtual poster*).
23. **Jacob R. Swartley**, Lauryn Power, Sara Makarem, David Green, and Kateri H. DuBay. Self Organization of Mixed Ligand Monolayers on Silver Nanoparticles. *ACS Fall National Meeting*, Atlanta, GA, August 2021 (*virtual poster*).
22. **Jessica K. Niblo** and Kateri H. DuBay. Modifying Assembly with Interparticle Potential Variation. *UVA ChemBio Seminar*, Charlottesville, VA, August 2020 (*talk*).
21. **Jacob R. Swartley**, Steven N. Merz, and Kateri H. DuBay. Modeling the Self-Assembly of Mixed-Ligand Monolayers on Ag Nanoparticles. *Berkeley Statistical Mechanics Meeting*, Berkeley, CA, January 2020 (*poster*).
20. **Steven Merz**, Zhongmin Zhang, Kateri H. DuBay. Using simulation to probe the sequence determinants within ATRP copolymerizations in bulk and on nanoparticle surfaces. *Berkeley Statistical Mechanics Meeting*, Berkeley, CA, January 2020 (*poster*).
19. **Qizhang Jia**, Cheng Yang, B. Jill Venton, and Kateri H. DuBay. Modeling the Surface Diffusion of Dopamine and Its Derivatives on Carbon Electrode Surfaces. *Berkeley Statistical Mechanics Meeting*, Berkeley, CA, January 2020 (*poster*).
18. **Zhongmin Zhang**, Kateri H. DuBay. Studying the effect of chain stiffness on sequence in step-growth copolymerization. *Berkeley Statistical Mechanics Meeting*, Berkeley, CA, January 2020 (*poster*).

17. **Jessica K Niblo**, **Jacob R Swartley**, **Zhongmin Zhang**, **Kateri H DuBay**. Self-Assembly of Viral Capsid-like Structures in an Oscillatory Energy Landscape. *Berkeley Statistical Mechanics Meeting*, Berkeley, CA, January 2020 (*poster*).
16. **Jacob R Swartley**, **Jessica Niblo**, and **Kateri H DuBay**. Self-Assembly of 2D Viral Capsids with Oscillatory Interactions. *Biophysical Society Annual Meeting*, Baltimore, MD, March 2019 (*poster*).
15. **Qizhang Jia**, **Xuanye Zhu**, **Austin H Cheng**, **Cory J Kim**, **Amy Y Wang**, and **Kateri H DuBay**. Studying the Folding Behavior of a 3D Lattice Protein Under Oscillatory Conditions. *Biophysical Society Annual Meeting*, Baltimore, MD, March 2019 (*poster*).
14. **Xuanye Zhu**, **Qizhang Jia**, and **Kateri H DuBay**. Protein Folding in a Lattice Model under Oscillatory Environment. *Biophysical Society Annual Meeting*, Baltimore, MD, March 2019 (*poster*).
13. **Austin H Cheng**, **Cory J Kim**, **Amy Y Wang**, **Xuanye Zhu**, **Qizhang Jia**, and **Kateri H DuBay**. Simulating the Folding States of Lattice Proteins Within an Oscillatory Environment. *Biophysical Society Annual Meeting*, Baltimore, MD, March 2019 (*poster*).
12. **Steven N Merz**, Zachary J Farrell, Joseph Pearring, Elise Hoover, Mark Kester, Sergei A Egorov, David L Green, and **Kateri H DuBay**. Investigations of Nanoparticle Monolayer Self-Assembly: Integrating MALDI-MS experiments with configurationally biased Monte Carlo simulations *Berkeley Statistical Mechanics Meeting*, Berkeley, CA, January 2019 (*poster*).
11. **Jessica K Niblo**, **Jacob Swartley**, **Zhongmin Zhang**, **Kateri H DuBay**. Shifting Self-Assembly Through Oscillations of Inter-Particle Interactions. *Berkeley Statistical Mechanics Meeting*, Berkeley, CA, January 2019 (*poster*).
10. **Zhongmin Zhang** and **Kateri H DuBay**. Investigating how nascent oligomer geometries and spatial heterogeneities influence the sequences of step-growth copolymers. *Berkeley Statistical Mechanics Meeting*, Berkeley, CA, January 2019. (*poster*)
9. **Steven Merz**, Zachary Farrell, Sergei Egorov, David Green and **Kateri H DuBay**. Design and Characterization of Ultrasmall Monolayer Protected Nanoparticles. *Squishy Materials Seminars*, UVA September 2018. (*talk*)
8. **Kyle N Plunkett**, Sambasiva Bheemireddy, Matthew P Hautzinger, Xinju Zhu, **Sambasivarao Somiseti**, **Kateri H DuBay**. *Conjugated polymers via cyclopentannulation strategies*. ACS National Meeting, New Orleans, LA, March 2018 (*talk*).
7. **Marcus Jordan**, **Zhongmin Zhang** and **Kateri H DuBay**. *Simulation of Free Radical Copolymerization for Nanoparticle Surface Functionalization*. UVA Summer Research Internship Program, UVA, Charlottesville, VA, August 2017 (*talk*).
6. **Marcus Jordan**, **Zhongmin Zhang** and **Kateri H DuBay**. Simulation of Nanoparticle Surface Functionalization via Free Radical Polymerization. Leadership Alliance National Symposium, Hartford, CT, July 2017 (*poster*).
5. **Zhongmin Zhang** and **Kateri H DuBay**. Modeling the influence of monomer properties on early-stage step growth copolymerizations. Berkeley Statistical Mechanics Meeting, Berkeley, CA, January 2017 (*poster*).
4. **Qizhang Jia**, Cheng Yang, B Jill Venton, and **Kateri H DuBay**. Atomistic simulations of dopamine on carbon microelectrode surfaces. Biophysical Society Meeting Meeting, New Orleans, LA, January 2017 (*poster*).
3. **Artemie Jurgenson** and **Kateri H DuBay**. NanoStar Poster Session, UVA, April 2017 (*poster*).
2. **Qizhang Jia**, Cheng Yang, B Jill Venton, and **Kateri H DuBay**. Atomistic simulations of dopamine on carbon microelectrode surfaces. Huskey Graduate Research Exhibition, UVA, March 2017 (*poster*).
1. **V. S. Somiseti** and **Kateri H DuBay**. Computational Study of the Horner-Wadsworth-Emmons Reactions for Their Reactivity and Selectivity. Fall National Meeting of the American Chemical Society, August 2015, Boston (*poster*).

CURRENT SUPPORT

Title: CAREER: Using numerical simulation to investigate of the influence of collective behaviors on the sequences of step-grown copolymers (CHE-1848009)

Sponsor: NSF

PI: K. H. DuBay
Dates of Contract Period: 4/1/2019-3/31/2024
Amount of Award: \$661,357

Title: Computational and Experimental Investigations of Phase-Separated Monolayers on Ultrasmall Noble Metal Nanoparticles (CHE-1904884)

Sponsor: **NSF**

PI: D. Green; Co-PI: K. H. DuBay

Dates of Contract Period: 8/1/2019 to 7/31/2022; NCE until 7/31/2023

Amount of Award: \$490,000 total; \$209,017 to DuBay Group

Title: Teaching Entropy and Modeling the Sequence-Determinants of Surface-Initiated Copolymerizations

Sponsor: **Research Corporation for Science Advancement, Cottrell Scholar Award**

PI: K. H. DuBay

Dates of Contract Period: 2020-2023

Amount of Award: \$100,000

Title: Characterizing the impact of emergent assembly on copolymer sequence (CNMS2023-A-01901)

Sponsor: **Oak Ridge National Lab – Center for Nanophase Materials Sciences: User Proposal**

PI: K. H. DuBay; Co-PIs: M. Chiu, R. Hamblin, W. Xu; Technical Contact: K. Hong

Dates of Contract Period: 2/1/2023-1/31/2024

Amount of Award: User Proposal

PRIOR SUPPORT

Title: Simulation-Informed Engineering of Polymer Surface Solvation for Water Desalination

Sponsor: **3 Cavaliers Program**

PI: K. H. DuBay; Co-PIs: R. Letteri and G. Geise

Dates of Contract Period: 6/1/2021 – 10/31/2022; NCE until 4/30/2023

Amount of Award: \$60,000; \$20,000 to DuBay Group

Title: Design, Development, and Testing of Innovative Point-of-Use Water Treatment Technologies

Sponsor: **3 Cavaliers Program**

PI: J. A. Smith; Co-PIs: K. H. DuBay and S. Sekhri

Dates of Contract Period: 1/1/2019 – 1/1/2020

Amount of Award: \$60,000

Title: Modeling the effect of an oscillatory cellular environment on protein folding

Sponsor: **Jeffress Foundation**

PI: K. H. DuBay

Dates of Contract Period: 6/30/2017 - 6/29/2018 (NCE to March 30, 2019)

Amount of Award: \$100,000

Title: UVA CHARGE Enhancement Fund

Sponsor: **UVA ADVANCE CHARGE Program**

PI: K. H. DuBay

Dates of Contract Period: Summer 2015 - Spring 2017

Amount of Award: \$4,800