Harold Wickes Hatch (a.k.a. Wick)

Chemical Engineer, National Institute of Standards and Technology

- Material Measurement Laboratory
- Chemical Sciences Division
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- 100 Bureau Dr., Gaithersburg, MD 20899-8320

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Education

Doctor of Philosophy, Princeton University, Princeton, NJ

- Chemical and Biological Engineering, 2014
- GPA: 3.95/4

Bachelor of Science in Engineering, Tulane University, New Orleans, LA

- Chemical and Biomolecular Engineering, 2008
- Double major Physics, minor Mathematics, summa cum laude
- GPA: 3.935/4

Fellowships and Scholarships

- National Research Council Postdoctoral Fellowship, 2013
- National Science Foundation Graduate Research Fellowship, 2010
- Princeton University Gordon Y. S. Wu Fellowship, 2008
- Barry M. Goldwater Scholarship, 2007
- Tulane University Founders Scholarship, 2003

Employment

Chemical Engineer, NIST, Gaithersburg, MD

- Chemical Informatics Research Group, Chemical Sciences Division, MML
- Simulating complex fluids using flat-histogram sampling methods and novel conformational sampling techniques
- Modeling monoclonal antibodies for applications in biomanufacturing
- Predicting thermodynamic properties of colloidal systems and self-assembling fluids for the design of new materials
- Writing molecular simulation programs and analysis code

Research Assistant, Princeton University, Princeton, NJ

- Chemical and Biological Engineering with Pablo G. Debenedetti, 2008-2013
- Proteins under tension
- Mechanical stresses on proteins in glassy matrices
- Chiral symmetry breaking in a microscopic model

Undergraduate Researcher, Tulane University, New Orleans, LA

- Chemical and Biomolecular Engineering with Henry S. Ashbaugh, 2006-2008
- Hydrophobic hydration of various water models
- Stability of model natively unfolded proteins

Undergraduate Researcher, Cornell University, Ithaca, NY

- Cornell Center for Materials Research REU with Paulette Q. Clancy, 2007
- Modeling methane hydrate stability

Tutor, Tulane University, New Orleans, LA

- Educational Resources Center, 2006-2008
- General Physics I and II, General and Organic Chemistry I and II, Calculus, Differential Equations and Linear Algebra

Publications

- https://www.nist.gov/publications/search_by_author/1165881
- https://scholar.google.com/citations?user=PUX35HgAAAAJ&hl=eni
- https://orcid.org/0000-0003-2926-9145

1. **"Colloidal Monolayers with Short-Range Attractions and Dipolar Repulsions"**, C. G. Yeh, H. W. Hatch, A. N. Sreenivasan, B. Bharti, V. K. Shen, Z. M. Sherman, T. M. Truskett, J. Phys. Chem. B, in submission, 2025.
2. **"Phase Equilibria of CO2 and n-Alkanes in Bulk and Confined Space Using Parallelized Wang-Landau Transition-Matrix Monte Carlo Simulations"**, J. Xu, H. W. Hatch, V. K. Shen, Z. Jin, Energy & Fuels, in press, 2025
    - https://doi.org/10.1021/acs.energyfuels.5c00420
3. **"Development of SAFT-Based Coarse-Grained Models of Carbon Dioxide and Nitrogen"**, A. Chremos, W. P. Krekelberg, H. W. Hatch, D. W. Siderius, N. A. Mahynski, V. K. Shen, J. Phys. Chem. B, in press, 2025.
    - https://doi.org/10.1021/acs.jpcb.5c00536
4. **"Extracting Orientation and Distance-Dependent Interaction Potentials between Proteins in Solutions Using Small-Angle X-ray/Neutron Scattering"**, Y. Liu, H. W. Hatch, G. Yuan, V. K. Shen, A. V. Grishaev, J. Panchal and M. Blanco, J. Phys. Chem. Lett., 15, 50, 12401-12407, 2024.
    - https://doi.org/10.1021/acs.jpclett.4c02629
5. **"Elucidating thermodynamically driven structure-property relations for zeolite adsorption using neural networks"**, C. Rzepa, D. Dabagian, D. W. Siderius, H. W. Hatch, V. K. Shen, J. Mittal and S. Rangarajan, JACS Au, 4, 12, 4673-4690, 2024.
    - https://doi.org/10.1021/jacsau.4c00429
6. **"Anisotropic coarse-grain Monte Carlo simulations of lysozyme, lactoferrin, and NISTmAb by precomputing atomistic models"**, H. W. Hatch, C. Bergonzo, M. A. Blanco, G. Yuan, S. Grudinin, M. Lund, J. E. Curtis, A. Grishaev, Y. Liu and V. K. Shen, J. Chem. Phys., 161, 9, 094113, 2024.

- https://doi.org/10.1063/5.0224809
- https://hhatch.com/papers/JCPv161n94113y2024.pdf

7. **"Monte Carlo molecular simulations with FEASST version 0.25.1"** H. W. Hatch, D. W. Siderius and V. K. Shen, J. Chem. Phys., 161, 9, 092501, 2024.
   - https://doi.org/10.1063/5.0224283
   - https://hhatch.com/papers/JCPv161n92501y2024.pdf
8. **"Flow Activation Energy of High-Concentration Monoclonal Antibody Solutions and Protein–Protein Interactions Influenced by NaCl and Sucrose"** G. Yuan, P F. Salipante, S. D. Hudson, R. E. Gillilan, Q. Huang, H. W. Hatch, V. K. Shen, A. V. Grishaev, S. Pabit, R. Upadhya, S. Adhikari, J. Panchal, M. A. Blanco and Y. Liu, Mol. Pharmaceutics, 21, 9, 4553, 2024.
   - https://doi.org/10.1021/acs.molpharmaceut.4c00460
9. **"Theory and Monte Carlo simulation of the ideal gas with shell particles in the canonical, isothermal-isobaric, grand canonical and Gibbs ensembles"** H. W. Hatch, V. K. Shen, and D. S. Corti, J. Chem. Phys., 161, 8, 084106, 2024.
   - https://doi.org/10.1063/5.0224305
   - https://hhatch.com/papers/JCPv161n084106y2024.pdf
10. **"Flat-Histogram Monte Carlo Simulation of Water Adsorption in Metal–Organic Frameworks"** D. W. Siderius, H. W. Hatch, V. K Shen, J. Phys. Chem. B, 128, 19, 4830-4845, 2024.
    - https://doi.org/10.1021/acs.jpcb.4c00753
    - https://tsapps.nist.gov/publication/get_pdf.cfm?pub_id=957246
11. **"Role of Domain-Domain Interactions on the Self-association and Physical Stability of Monoclonal Antibodies: Effect of pH and Salt"** A. Y. Xu, M. A. Blanco, M. M. Castellanos, C. W. Meuse, K. Mattison, I. Karageorgos, H. W. Hatch, V. K. Shen, J. E. Curtis, J. Phys. Chem. B, 127, 39, 8344-8357, 2023.
    - https://doi.org/10.1021/acs.jpcb.3c03928
12. **"pH response of sequence-controlled polyampholyte brushes"** X. Yuan, H. W. Hatch, J. C. Conrad, A. B. Marciel, J. C. Palmer, Soft Matter, 19, 4333-4344, 2023.
    - https://doi.org/10.1039/D3SM00447C
    - https://tsapps.nist.gov/publication/get_pdf.cfm?pub_id=936679
13. **"Efficiency Comparison of Single- and Multiple-Macrostate Grand Canonical Ensemble Transition-Matrix Monte Carlo Simulations"** H. W. Hatch, D. W. Siderius, J. R. Errington and V. K. Shen, J. Phys. Chem. B, 127, 3041-3051, 2023.
    - https://doi.org/10.1021/acs.jpcb.3c00613
    - https://hhatch.com/papers/JCPv127y2023.pdf
14. **"Temperature Extrapolation of Henry's Law Constants and the Isosteric Heat of Adsorption"** D. W. Siderius, H. W. Hatch, V. K. Shen, J. Phys. Chem. B, 126, 7999-8009, 2022.
    - https://doi.org/10.1021/acs.jpcb.2c04583
    - https://tsapps.nist.gov/publication/get_pdf.cfm?pub_id=935037
15. **"Comments on "Monte Carlo Simulations for Water Adsorption in Porous Materials: Best Practices and New Insights""** D. W. Siderius, H. W. Hatch, J. R. Errington and V. K. Shen, AIChE J., 2022.
    - https://doi.org/10.1002/aic.17686
16. **"Extrapolation and interpolation strategies for efficiently estimating structural observables as a function of temperature and density"** J. I. Monroe, H. W. Hatch, N. A. Mahynski, M. S. Shell and V. K. Shen, J. Chem. Phys., 153, 144101, 2020.

- https://doi.org/10.1063/5.0014282
- https://tsapps.nist.gov/publication/get_pdf.cfm?pub_id=930298

17. **"Parallel Prefetching for Canonical Ensemble Monte Carlo Simulations"** H. W. Hatch, J. Phys. Chem. B, 124, 7191, 2020.
    - https://doi.org/10.1021/acs.jpca.0c05242
    - https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7808336/
18. **"Computational Investigation of Correlations in Adsorbate Entropy for Pure-Silica Zeolite Adsorbents"** C. Rzepa, D. W. Siderius, H. W. Hatch, V. K. Shen, S. Rangarajan and J. Mittal, J. Phys. Chem. C, 124, 163350-16361, 2020.
    - https://doi.org/10.1021/acs.jpcc.0c02671
    - https://tsapps.nist.gov/publication/get_pdf.cfm?pub_id=930106
19. **"Flat-histogram extrapolation as a useful tool in the age of big data"** N. A. Mahynski, H. W. Hatch, M. Witman, D. A. Sheen, J. R. Errington and V. K. Shen, Mol. Sim., 47, 2020.
    - https://doi.org/10.1080/08927022.2020.1747617
    - https://tsapps.nist.gov/publication/get_pdf.cfm?pub_id=929154
20. **"Dynamic arrest of adhesive hard rod dispersions"** R. P. Murphy, H. W. Hatch, N. A. Mahynski, V. K. Shen, N. J. Wagner, Soft Matter, 16, 1279, 2020.
    - https://doi.org/10.1039/C9SM01877H
    - https://tsapps.nist.gov/publication/get_pdf.cfm?pub_id=925778
21. **"Tabular potentials for Monte Carlo simulation of supertoroids with short range interactions"** H. W. Hatch and G. W. McCann, J. Res. NIST, 124, 124032, 2019.
    - https://doi.org/10.6028/jres.124.032
22. **"Improving the efficiency of Monte Carlo simulations of ions using expanded grand canonical ensembles"** H. W. Hatch, S. W. Hall, J. R. Errington and V. K. Shen, J. Chem. Phys., 161, 144109, 2019.
    - https://doi.org/10.1063/1.5123683
    - https://tsapps.nist.gov/publication/get_pdf.cfm?pub_id=928337
23. **"Designing molecular building blocks for the self-assembly of complex porous networks"** T.A. Maula, H. W. Hatch, V. K. Shen, S. Rangarajan, and J. Mittal, Mol. Sys. Des. Eng., 4, 644, 2019.
    - https://doi.org/10.1039/C9ME00006B
    - https://tsapps.nist.gov/publication/get_pdf.cfm?pub_id=927382
24. **"Evaluating the Effects of Hinge Flexibility on the Solution Structure of Antibodies at Concentrated Conditions"** M. A. Blanco, H. W. Hatch, J. E. Curtis, V. K. Shen, J. Pharm. Sci, 108, 1663-1674, 2019.
    - https://doi.org/10.1016/j.xphs.2018.12.013
    - https://tsapps.nist.gov/publication/get_pdf.cfm?pub_id=926491
25. **"Monte Carlo simulation of cylinders with short-range attractions"** H. W. Hatch, N. A. Mahynski, R. P. Murphy, M. A. Blanco, and V. K. Shen, AIP Advances, 8, 095210, 2018.
    - https://doi.org/10.1063/1.5040252
26. **"A methodology to calculate small-angle scattering profiles of macromolecular solutions from molecular simulations in the grand-canonical ensemble"** M. A. Blanco, H. W. Hatch, J. E. Curtis, and V. K. Shen, J. Chem. Phys., 149, 084203, 2018.
    - https://doi.org/10.1063/1.5029274

27. **"Assembly of three-dimensional binary superlattices from multi-flavored particles"** E. Pretti, H. Zerze, M. Song, Y. Ding, N. A. Mahynski, H. W. Hatch, V. K. Shen, and J. Mittal, Soft Matter, 14, 6303, 2018.
    - https://doi.org/10.1039/C8SM00989A
    - https://tsapps.nist.gov/publication/get_pdf.cfm?pub_id=925282
28. **"Predicting structural properties of fluids by thermodynamic extrapolation"** N. A. Mahynski, S. Jiao, H. W. Hatch, M. A. Blanco, and V. K. Shen, J. Chem. Phys., 148, 194105, 2018.
    - https://doi.org/10.1063/1.5026493
29. **"FEASST: Free Energy and Advanced Sampling Simulation Toolkit"** H. W. Hatch, N. A. Mahynski, V. K. Shen, J. Res. Natl. Inst. Stan., 123, 123004, 2018.
    - https://doi.org/10.6028/jres.123.004
30. **"Communication: Predicting virial coefficients and alchemical transformations by extrapolating Mayer-sampling Monte Carlo simulations"** H. W. Hatch, S. Jiao, N. A. Mahynski, M. A. Blanco, V. K. Shen, J. Chem. Phys., 147, 231102, 2017.
    - https://doi.org/10.1063/1.5016165
31. **"NIST Standard Reference Simulation Website"** V. K. Shen, D.W. Siderius, W. P. Krekelberg, and H. W. Hatch, Eds., NIST Standard Reference Database Number 173, National Institute of Standards and Technology, Gaithersburg MD, 20899
    - https://doi.org/10.18434/T4M88Q
32. **"Assembly of multi-flavored two-dimensional colloidal crystals"** N. A. Mahynski, H. Zerze, H. W. Hatch, V. K. Shen and J. Mittal, Soft Matter, 13, 5397-5408, 2017.
    - https://doi.org/10.1039/C7SM01005B
    - https://tsapps.nist.gov/publication/get_pdf.cfm?pub_id=922982
33. **"Molecular dynamics simulation of trimer self-assembly under shear"** R.D. Mountain, H. W. Hatch and V. K. Shen, Fluid Phase Equilibria, 440, 87-94, 2017.
    - https://dx.doi.org/10.1016/j.fluid.2017.02.017
    - https://hhatch.com/papers/FPEv440p87y2017.pdf
34. **"Depletion-driven crystallization of cubic colloids sedimented on a surface"** H. W. Hatch, W. P. Krekelberg, S. D. Hudson and V. K. Shen, J. Chem. Phys., 144, 194902, 2016.
    - https://dx.doi.org/10.1063/1.4949758
    - https://hhatch.com/papers/JCPv144n194902y2016.pdf
35. **"Self-assembly of trimer colloids: effect of shape and interaction range"** H. W. Hatch, S. Y. Yang, J. Mittal and V. K. Shen, Soft Matter, 12, 4170-4179, 2016.
    - https://dx.doi.org/10.1039/C6SM00473C
    - https://tsapps.nist.gov/publication/get_pdf.cfm?pub_id=919870
    - https://hhatch.com/papers/C6SM00473C.pdf
36. **"Computational study of trimer self-assembly and fluid phase behavior"** H. W. Hatch, J. Mittal and V. K. Shen, J. Chem. Phys., 142, 164901, 2015.
    - https://dx.doi.org/10.1063/1.4918557
    - https://hhatch.com/papers/JCPv142n164901y2015.pdf
37. **"Computational Study of the Stability of the Miniprotein Trp-Cage, the GB1 β-Hairpin, and the AK16 Peptide, under Negative Pressure"** H. W. Hatch, F. H. Stillinger and P. G. Debenedetti, J. Phys. Chem. B, 118, 7761-7769, 2014.
    - https://dx.doi.org/10.1021/jp410651u

38. **"Molecular modeling of mechanical stresses on proteins in glassy matrices: Formalism"** H. W. Hatch and P. G. Debenedetti, J. Chem. Phys., 137, 035103, 2012.
    - https://dx.doi.org/10.1063/1.4734007
    - https://hhatch.com/papers/JCPv137n035103.pdf
39. **"Chiral symmetry breaking in a microscopic model with asymmetric autocatalysis and inhibition"** H. W. Hatch, F.H. Stillinger and P. G. Debenedetti, J. Chem. Phys., 133, 224502, 2010.
    - https://dx.doi.org/10.1063/1.3511715
    - https://hhatch.com/papers/JCPv133n224502.pdf
40. **"Assessing the thermodynamic signatures of hydrophobic hydration for several common water models"** H. S. Ashbaugh, N. J. Collett, H. W. Hatch, J. A. Staton, J. Chem. Phys., 132, 124504, 2010.
    - https://dx.doi.org/10.1063/1.3366718
    - https://hhatch.com/papers/JCPv132n124504.pdf
41. **"Natively unfolded protein stability as a coil-to-globule transition in charge/hydropathy space"** H. S. Ashbaugh and H. W. Hatch, J. Amer. Chem. Soc., 130, 9536, 2008.
    - https://dx.doi.org/10.1021/ja802124e

Invited Presentations

All presentations listed here were presented by H. W. Hatch.

1. **"Multiscale Modeling of Monoclonal Antibodies in High Concentration Formulations,"** H. W. Hatch, C. Bergonzo, G. Yuan, M. Lund, S. Grudinin, A. V. Grishaev, Y. Liu and V. K. Shen, Stevens Institute of Technology Department of Chemical Engineering and Materials Science Seminar Series, October 2024
    - https://www.stevens.edu/school-engineering-science/departments/chemical-engineering-materials-science/seminars
2. **"Multiscale Modeling of Monoclonal Antibodies in High Concentration Formulations,"** H. W. Hatch, C. Bergonzo, V. Burns Casamayor, G. Yuan, A. V. Grishaev, Y. Liu and V. K. Shen, STMS seminar, 2024
    - https://sites.google.com/view/stms2021/schedule
3. **"Multiscale Modeling of Monoclonal Antibodies in High Concentration Formulations,"** H. W. Hatch, C. Bergonzo, V. Burns Casamayor, G. Yuan, A. V. Grishaev, Y. Liu and V. K. Shen, WEBINAR: Antibodies in Solution: a LINXS - NIST Webinar Series, 2023.
    - https://www.linxs.se/events/webinar-antibodies-in-solution-a-linxscgsimulations
4. **"Multiscale Modeling of Monoclonal Antibodies in High Concentration Formulations,"** H. W. Hatch, C. Bergonzo, V. Burns Casamayor, G. Yuan, A. V. Grishaev, Y. Liu and V. K. Shen, Department of Chemical Engineering Seminar, University of Arkansas, Fayetteville AR, 2023.
    - https://chemical-engineering.uark.edu/academics/graduate-program/seminar.php
5. **"Multiscale Modeling of Monoclonal Antibodies in High Concentration Formulations,"** H. W. Hatch, C. Bergonzo, V. Burns Casamayor, G. Yuan, A. V. Grishaev, Y. Liu and V. K. Shen, Liquids, Glasses and Other Adventures in Thermodynamics and Statistical Mechanics, Princeton University, Princeton NJ, 2023.
    - https://pgd70.princeton.edu/
6. **"Simulations of concentrated solutions of monoclonal antibodies and sticky cylindrical particles using open-source software,"** H. W. Hatch, R. Murphy, M. A. Blanco, N. A. Mahynski, J. E. Curtis, V. K. Shen, CECAM simSAS, ILL, Grenoble, France, 2019
    - https://workshops.ill.fr/event/143/page/141-programme-titles-abstracts

7. **"Improving reproducibility of molecular simulations with reference data and open source software."** H. W. Hatch, D. W. Siderius, V. K. Shen, American Chemical Society Annual Meeting, Orlando, Florida, 2019
    - https://molssi.org/2019/03/18/molssi-sustainable-software-symposium-at-spring-2019-acs-meeting/
8. **"Theoretical and Computational Studies of the Mechanical Stability of Proteins, and Colloidal Self-Assembly."** H. W. Hatch, ExxonMobil Research & Engineering Company, Annandale, New Jersey, 2015.
9. **"Molecular Modeling of the Mechanical Stability of Proteins, and of the Origin of Biological Homochirality."** H. W. Hatch, F. H. Stillinger, P. G. Debenedetti, National Institutes of Health, NIDDK, Laboratory of Chemical Physics, Bethesda, Maryland, 2013.
10. **"Molecular Modeling of the Mechanical Stability of Proteins, and of the Origin of Biological Homochirality."** H. W. Hatch, F. H. Stillinger, P. G. Debenedetti, National Institute of Standards and Technology, Chemical Sciences Division, Gaithersburg, Maryland, 2013.
11. **"Molecular Modeling of the Mechanical Stability of Proteins, and of the Origin of Biological Homochirality."** H. W. Hatch, F. H. Stillinger, P. G. Debenedetti, University of California, Santa Barbara, Department of Chemical Engineering, Santa Barbara, California, 2013.

Oral Presentations

All presentations listed here were presented by H. W. Hatch.

1. **"Molecular Simulation Applications in Pharmaceuticals and Carbon Capture,"** H. W. Hatch, Daniel W. Siderius, Vincent K. Shen, Tour for UMD Chemistry Olympiad Study Camp, NIST, Gaithersburg, MD, 2024.
2. **"Multiscale Modeling of Monoclonal Antibodies in High Concentration Formulations,"** H. W. Hatch, C. Bergonzo, V. Burns Casamayor, G. Yuan, A. V. Grishaev, Y. Liu and V. K. Shen, 23rd MASM: The Mid-Atlantic Soft Matter Workshop, Georgetown University, Washington, D.C., 2024.
3. **"Multiscale Modeling of Monoclonal Antibodies in High Concentration Formulations,"** H. W. Hatch, C. Bergonzo, V. Burns Casamayor, G. Yuan, A. V. Grishaev, Y. Liu and V. K. Shen, American Institute of Chemical Engineers Annual Meeting, Orlando, Florida, 2023.
4. **"Parallelization of Grand Canonical Ensemble Monte Carlo Using Prefetching and Windowing of Flat Histogram Simulations"** H. W. Hatch and V. K. Shen, American Institute of Chemical Engineers Annual Meeting, Pheonix, Arizona, 2022.
5. **"Parallelization of Monte Carlo Simulations using Prefetching"** H. W. Hatch, V. K. Shen, 21st Symposium on Thermophysical Properties, Boulder, Colorado, 2021
6. **"Improving the efficiency of Monte Carlo simulations of ions using expanded grand canonical ensembles"** H. W. Hatch, S. W. Hall, J. R. Errington and V. K. Shen, American Institute of Chemical Engineers Annual Meeting, Orlando, Florida, 2019
7. **"Monte Carlo Simulation of Cylinders with Short-Range Attractions"** H. W. Hatch, N. A. Mahynski, R. Murphy, M. A. Blanco and V. K. Shen, American Institute of Chemical Engineers Annual Meeting, Orlando, Florida, 2019
8. **"Predicting virial coefficients and alchemical transformations by extrapolating Mayer-sampling Monte Carlo simulations"** H. W. Hatch, S. Jiao, N. A. Mahynski, M. A. Blanco, V. K. Shen, American Institute of Chemical Engineers Annual Meeting, Pittsburg, Pennsylvania, 2018
9. **"FEASST: Free Energy and Advanced Sampling Simulation Toolkit"** H. W. Hatch, N. A. Mahynski, V. K. Shen, Twentieth Symposium on Thermophysical Properties, Boulder, Colorado, 2018
10. **"Predicting virial coefficients and alchemical transformations by extrapolating Mayer-sampling Monte Carlo simulations"** H. W. Hatch, S. Jiao, N. A. Mahynski, M. A. Blanco, V. K. Shen, Twentieth Symposium on Thermophysical Properties, Boulder, Colorado, 2018

11. **"Computer simulation of cylinders with short-ranged attractive interactions"** H. W. Hatch, R. P. Murphy, N. A. Mahynski, V. K. Shen and N. J. Wagner, 91st ACS Colloid and Surface Science Symposium, The City College of New York, New York, 2017
12. **"Computational Studies of the Depletion-Driven Self-Assembly of Patchy Trimer Colloids and Cubic Colloids"** H. W. Hatch, W. P. Krekelberg, J. Mittal, S. D. Hudson and V. K. Shen, 90th ACS Colloid and Surface Science Symposium, Harvard University, Cambridge, Massachusetts, 2016
13. **"Computational Study of Coarse-Grained Models for Monoclonal Antibodies"** H. W. Hatch, Y. Ding, J. Mittal and V. K. Shen, American Institute of Chemical Engineers Annual Meeting, Hilton Atlanta, Atlanta, Georgia, 2014
14. **"Thermodynamics and simulation of the negative pressure folding and unfolding of trp-cage and GB1 beta-hairpin miniproteins"** H. W. Hatch, F. H. Stillinger and P. G. Debenedetti, American Institute of Chemical Engineers Annual Meeting, Hilton San Francisco Union Square, San Francisco, California, 2013
15. **"Molecular Modeling of Mechanical Stresses on Proteins in Glassy Carbohydrate-Water Matrices"** H. W. Hatch, and P. G. Debenedetti, Chemical and Biological Engineering Graduate Student Symposium, Princeton University, Princeton, New Jersey, 2011
16. **"Molecular Modeling of Mechanical Stresses on Proteins in Glassy Carbohydrate-Water Matrices"** H. W. Hatch, and P. G. Debenedetti, American Institute of Chemical Engineers Annual Meeting, Minneapolis Convention Center, Minneapolis, Minnesota, 2011
17. **"Microscopic Models of Chiral Amplification and Symmetry Breaking"** H. W. Hatch, T. G. Lombardo, F. H. Stillinger and P. G. Debenedetti, American Institute of Chemical Engineers Annual Meeting, Salt Palace Convention Center, Salt Lake City, Utah, 2010
18. **"Computational studies of Mechanical Stresses on Proteins in the Glassy State"** H. W. Hatch, and P. G. Debenedetti, American Institute of Chemical Engineers Annual Meeting, Salt Palace Convention Center, Salt Lake City, Utah, 2010
19. **"Stability of Natively Unfolded Proteins"** H. W. Hatch and H. S. Ashbaugh, AIChE Southern Regional Conference, Auburn University, Auburn, Alabama 2008
20. **"Simulation of Type I Methane Hydration using the Fluctuating Charge Model"** H. W. Hatch and P. Q. Clancy, Cornell Center for Materials Research Colloquium Paper, Cornell University, Ithaca, New York 2007

Poster Presentations

All presentations listed here were presented by H. W. Hatch.

1. **"Uncertainty Quantification in Transition-Matrix Monte Carlo Simulations"** H. W. Hatch, D. W. Siderius, A. Brady-Mine and V. K. Shen, American Institute of Chemical Engineers Annual Meeting, Virtual, 2021
2. **"Parallel Prefetching for Canonical Ensemble Monte Carlo Simulation"** H. W. Hatch, American Institute of Chemical Engineers Annual Meeting, Virtual, 2020
3. **"Monte Carlo simulations of monoclonal antibodies, rods, cubes and patchy particles"** H. W. Hatch, Gordon Research Conference: Colloidal, Macromolecular & Polyelectrolyte Solutions, Four Points Sheraton, Ventura, California, 2020
4. **"FEASST: Free Energy and Advanced Sampling Simulation Toolkit"** H. W. Hatch, N. A. Mahynski, V. K. Shen, American Institute of Chemical Engineers Annual Meeting, Pittsburg, Pennsylvania, 2018
5. **"Predicting virial coefficients and alchemical transformations by extrapolating Mayer-sampling Monte Carlo simulations"** H. W. Hatch, S. Jiao, N. A. Mahynski, M. A. Blanco, V. K. Shen, Foundations of Molecular Modeling and Simulation, Delavan, Wisconsin, 2018
6. **"Predicting virial coefficients and alchemical transformations by extrapolating Mayer-sampling Monte Carlo simulations"** H. W. Hatch, S. Jiao, N. A. Mahynski, M. A. Blanco, V. K. Shen, Gordon

Research Conference: Colloidal, Macromolecular & Polyelectrolyte Solutions, Four Points Sheraton, Ventura, California, 2018

7. **"Computer simulation of cylinders with short-ranged attractive interactions"** H. W. Hatch, R. P. Murphy, N. A. Mahynski, V. K. Shen and N. J. Wagner, Gordon Research Conference: Liquids, Chemistry and Physics of, Holderness, New Hampshire, 2017
8. **"Computational Studies of the Depletion-Driven Self-Assembly of Patchy Trimer Colloids and Cubic Colloids"** H. W. Hatch, W. P. Krekelberg, J. Mittal, S. D. Hudson and V. K. Shen, CCP-SAS Project Workshop, NIST Center for Neutron Research, Gaithersburg, Maryland, 2016
9. **"Computational Studies of the Depletion-Driven Self-Assembly of Patchy Trimer Colloids and Cubic Colloids"** H. W. Hatch, W. P. Krekelberg, J. Mittal, S. D. Hudson and V. K. Shen, Gordon Research Conference: Colloidal, Macromolecular & Polyelectrolyte Solutions, Four Points Sheraton, Ventura, California, 2016
10. **"Computational Study of Coarse- Grained Models for Monoclonal Antibodies"** H. W. Hatch, Y. Ding, J. Mittal and V. K. Shen, Gordon Research Conference: Water and Aqueous Solutions, Holderness School, Holderness, New Hampshire, 2014
11. **"Negative Pressure Folding and Unfolding Simulations of Trp-cage and GB1 Beta-hairpin Miniproteins"** H. W. Hatch, and P. G. Debenedetti, Gordon Research Conference: Chemistry and Physics of Liquids, Holderness School, Holderness, New Hampshire, 2013
12. **"Molecular Modeling of Mechanical Stresses on Proteins in Glassy Matrices"** H. W. Hatch, and P. G. Debenedetti, Gordon Research Conference: Water and Aqueous Solutions, Holderness School, Holderness, New Hampshire, 2012
13. **"Molecular Modeling of Mechanical Stresses on Proteins in Glassy Matrices"** H. W. Hatch, and P. G. Debenedetti, Gordon-Kenan Research Seminar: Water and Aqueous Solutions, Holderness School, Holderness, New Hampshire, 2012
14. **"Microscopic Models of Chiral Amplification and Symmetry Breaking"** H. W. Hatch, T. G. Lombardo, F. H. Stillinger and P. G. Debenedetti, Gordon Research Conference: Water and Aqueous Solutions, Holderness School, Holderness, New Hampshire, 2010
15. **"Water-like Dynamic Anomalies in a Repulsive Spherical Model"** H. W. Hatch, Princeton Research Symposium, Princeton University, Princeton, New Jersey 2008

Software

1. **FEASST**: Free Energy and Advanced Sampling Simulation Toolkit
    - Open source C++11 software to conduct molecular and particle-based simulations with flat-histogram Monte Carlo and molecular dynamics methods.
    - Python interface.
    - https://pages.nist.gov/feasst/
    - https://github.com/usnistgov/feasst
    - https://doi.org/10.6028/jres.123.004
    - https://doi.org/10.18434/M3S095
    - As of 2022, over 77 thousand lines of C++ source code with 24 GitHub stars.
2. **mayer-extrapolation**
    - Use extrapolation of Mayer-sampling Monte Carlo to obtain virial coefficients
    - https://github.com/usnistgov/mayer-extrapolation
    - https://doi.org/10.1063/1.5016165

Computer Skills

Programming Languages: C++, python, FORTRAN, bash, LaTeX

Software Engineering

- Revision control: Git
- Unit testing: Google, Python
- Documentation: Sphinx, Doxygen, MD, RST
- Debug: Valgrind, GDB
- CMake, Make, Coverage, Linters

High Performance Computer Cluster Building and Administration

- Built and installed CPU and GPU rack-mounted nodes at NIST
- Ubuntu, Rocky, PUIAS Linux, Rocks, Windows Server
- Built and administrated PGD Group HPC Cluster (3.5+ million CPU hours utilized)

Website Administration

- FEASST, NIST SRSW, PGD, PGD Group and hhatch.com

Other Software

- Jupyter, Pandas, MATLAB, Mathematica, Gnuplot, Microsoft Office, Zotero

Available Opportunities

- For current graduate students, contact me about applying for the NIST NRC RAP Fellowship Opporunity 1 or 2
- For current undergraduate students, contact me about applying for NIST SURF: https://www.nist.gov/surf
- Guest researcher and postdocs: please email me for more opportunities.

Mentorship

1. **Samiha Sharlin**, UMBC / NIST Guest Researcher, 2024
    - Monte Carlo simulations of adsorption.
2. **Violetta Burns**, IBBR postdoc, 2023
    - Molecular dynamics simulations of all-atom and coarse-grained monoclonal antibodies in solution.
    - https://scholar.google.com/citations?user=3pNUxEYAAAAJ&hl=en&oi=ao
    - https://orcid.org/0000-0003-3732-0641
3. **Alexandria Brady-Mine**, Summer Undergraduate Research Fellow, 2021
    - Studied uncertainty quantification in Transition-Matrix Monte Carlo simulations.
    - Subsequently 2022 Barry Goldwater Scholar, 2022 Rhodes finalist and 2023 NSF GRFP fellow.
    - Currently working with Dr. Elazer Edelman at the Harvard-MIT Biomedical Engineering Center in pursuit of Masters and Ph.D.
4. **Steven Hall**, Summer Undergraduate Research Fellow, 2018

- Subsequently chemical engineering graduate student at Clemson University and the University of Minnesota under the mentorship of Professor Sapna Sarupria.
- https://doi.org/10.1063/1.5123683

5. **Kamryn Kant**, Summer Undergraduate Research Fellow, 2018
    - Subsequently chemical engineering graduate student at Clemson University under the mentorship of Professor Sapna Sarupria.
6. **Sally Jiao**, Summer Undergraduate Research Fellow, 2017 and 2018
    - Studied thermodynamic extrapolation of structural properties and virial coefficients.
    - https://doi.org/10.1063/1.5026493
    - https://doi.org/10.1063/1.5016165
    - Subsequently received the 2018 NSF Graduate Research Fellowship.
    - Subsequently chemical engineering graduate student at the University of California, Santa Barbara under the mentorship of Professor M. Scott Shell.
    - Currently an engineer at Eli Lilly.
7. **Gordon W. McCann**, Summer Undergraduate Research Fellow, 2016
    - Studied supertoroid-shaped particles.
    - https://doi.org/10.6028/jres.124.032
    - Subsequently physics graduate student at Florida State University under the mentorship of Professor Ingo Wiedenhoever.
8. **Seung-Yeob Yang**, Montegomery College/MML Internship, 2015
    - Studied self-assembly of patchy particles.
    - https://doi.org/10.1039/C6SM00473C
    - Subsequently obtained a degree in Mechanical Engineering at the University of Maryland.
    - Project Engineer at HBW Construction.

Professional Activities

- **Organization of Technical Conferences**
    1. American Institute of Chemical Engineers, Annual Meeting, Fall 2022, Engineering Sciences and Fundamentals, Thermophysical Properties and Phase Behavior Co-chair.
    2. American Institute of Chemical Engineers, Annual Meeting, Fall 2021, Engineering Sciences and Fundamentals, Thermophysical Properties and Phase Behavior Co-chair.
    3. American Institute of Chemical Engineers, Annual Meeting, Fall 2020, Computational Molecular Science and Engineering Forum, Applications of Molecular Modeling to Study Interfacial Phenomena Chair/Co-chair.
    4. American Institute of Chemical Engineers, Annual Meeting, Fall 2019, Computational Molecular Science and Engineering Forum, Applications of Molecular Modeling to Study Interfacial Phenomena Chair/Co-chair.
    5. NIST MML Chemical Sciences Division Research Day, May 2019, Organizing committee.
    6. American Institute of Chemical Engineers, Annual Meeting, Fall 2018, Computational Molecular Science and Engineering Forum, Applications of Molecular Modeling to Study Interfacial Phenomena Co-chair.
    7. Princeton Research Symposium 2009, Organizing committee.

- **Reviewer**
    1. Journal of Chemical Physics
    2. Journal of Physical Chemistry
    3. Journal of Chemical Theory and Computation
    4. Journal of Theoretical and Computational Chemistry
    5. Journal of Applied Physics
    6. Living Journal of Computational Molecular Science
    7. PLOS ONE
- Near-Peer Mentor, NSF Molecular Biophysics REU, Princeton University, 2011
- Member, Tau Beta Pi
- Member, Phi Beta Kappa

Awards and Honors

Princeton University

- Schowalter Travel Award, 2011
- Gordon Research Conference Travel Award, 2010
- School of Engineering and Applied Science Commendation for Outstanding Teaching, 2010
- Interview for Hertz Graduate Fellowship, 2009

Tulane University

- Practice School Award, 2008
- AIChE Achievement Award for Highest GPA in Class, 2007
- Provost's Fund for Faculty/Student Scholarly Engagement, 2006

Auburn University

- Prio Prize for Academic Excellence in Chemical Engineering, 2005

Teaching Experience

Princeton University

- Assistant in Instruction, CBE 503 Advanced Thermodynamics, Fall 2011
- Assistant in Instruction, CBE 246 Thermodynamics, Spring 2010

Tulane University

- Tutor in Math, Physics and Chemistry, 2006-2008

Research Interests

- Statistical Mechanics Theory and Molecular Simulation Methods
- Colloidal Self-Assembly
- Protein-Protein Interactions, Protein Aggregation, Folding, Stability and Biopreservation
- Hydrophobic Hydration