

Harold Wickes Hatch (known as Wick)**Chemical Engineer****Curriculum vitae**

National Institute of Standards and Technology
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Education

Doctor of Philosophy, Princeton University, Princeton, NJ 2014
Chemical and Biological Engineering GPA 3.95/4

Bachelor of Science in Engineering, Tulane University, New Orleans, LA 2008
Chemical and Biomolecular Engineering GPA 3.935/4
Double major Physics, minor Mathematics , *summa cum laude*

Research Experience

Chemical Engineer, NIST, Gaithersburg, MD 2013-present
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
- Developing software tools for bench scientists to design experiments and analyze results

Research Assistant, Princeton University, Princeton, NJ 2008-2013
Chemical and Biological Engineering with Pablo G. Debenedetti

- Proteins under tension
- Mechanical stresses on proteins in glassy matrices
- Chiral symmetry breaking in a microscopic model

Undergraduate Researcher, Tulane University, New Orleans, LA 2006-2008
Chemical and Biomolecular Engineering with Henry S. Ashbaugh

- Hydrophobic hydration of various water models
- Stability of model natively unfolded proteins

Undergraduate Researcher, Cornell University, Ithaca, NY Summer 2007
Cornell Center for Materials Research REU with Paulette Q. Clancy

- Modeling methane hydrate stability

Teaching Experience

Princeton University
Assistant in Instruction, CBE 503 Advanced Thermodynamics Fall 2011

Assistant in Instruction, CBE 246 Thermodynamics

Spring 2010

Tulane University Educational Resources and Counseling

Tutor in Math, Physics and Chemistry

2006-2008

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

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
MGE@MSA/WAESO Research Conference Third Place Poster	2006

Auburn University

Prio Prize for Academic Excellence in Chemical Engineering	2005
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Professional Organizations and Activities

Near-Peer Mentor, NSF Molecular Biophysics REU, Princeton University	2011
Organizing Committee, Princeton Research Symposium	2009
Member, Tau Beta Pi	2008-present
Member, Phi Beta Kappa	2008-present
Member, American Institute of Chemical Engineers	2007-present

Research Interests

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

Publications

10. "Assembly of multi-flavored two-dimensional colloidal crystals" N.A. Mahynski, H. Zerze, **H. W. Hatch**, V.K. Shen and J. Mittal, *in preparation*, 2017.

9. "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.
<http://dx.doi.org/10.1016/j.fluid.2017.02.017>
<http://hhatch.com/papers/FPEv440p87y2017.pdf>
8. "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.
<http://dx.doi.org/10.1063/1.4949758>
<http://hhatch.com/papers/JCPv144n194902y2016.pdf>
7. "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.
<http://dx.doi.org/10.1039/C6SM00473C>
<http://hhatch.com/papers/C6SM00473C.pdf>
6. "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.
<http://dx.doi.org/10.1063/1.4918557>
<http://hhatch.com/papers/JCPv142n164901y2015.pdf>
5. "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.
<http://dx.doi.org/10.1021/jp410651u>
4. "Molecular modeling of mechanical stresses on proteins in glassy matrices: Formalism" **H. W. Hatch** and P. G. Debenedetti, *J. Chem. Phys.*, 137, 035103, 2012.
<http://dx.doi.org/10.1063/1.4734007>
<http://hhatch.com/papers/JCPv137n035103.pdf>
3. "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.
<http://dx.doi.org/10.1063/1.3511715>
<http://hhatch.com/papers/JCPv133n224502.pdf>
2. "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.
<http://dx.doi.org/10.1063/1.3366718>
<http://hhatch.com/papers/JCPv132n124504.pdf>
1. "Natively unfolded protein stability as a coil-to-globule transition in charge/hydrophobicity space" H. S. Ashbaugh and **H. W. Hatch**, *J. Amer. Chem. Soc.*, 130, 9536, 2008.
<http://dx.doi.org/10.1021/ja802124e>

Presentations

#Oral; *Poster; Presenter Bolded

18. **H. W. Hatch**, W. P. Krekelberg, J. Mittal, S. D. Hudson and V. K. Shen, "Computational Studies of the Depletion-Driven Self-Assembly of Patchy Trimer Colloids and Cubic Colloids" 90th ACS Colloid & Surface Science Symposium, Harvard University, Cambridge, Massachusetts, 2016[#]

17. **H. W. Hatch**, W. P. Krekelberg, J. Mittal, S. D. Hudson and V. K. Shen, "Computational Studies of the Depletion-Driven Self-Assembly of Patchy Trimer Colloids and Cubic Colloids" Gordon Research Conference: Colloidal, Macromolecular & Polyelectrolyte Solutions, Four Points Sheraton, Ventura, California, 2016^{*}

16. **H. W. Hatch**, Y. Ding, J. Mittal and V. K. Shen, "Computational Study of Coarse-Grained Models for Monoclonal Antibodies" American Institute of Chemical Engineers Annual Meeting, Hilton Atlanta, Atlanta, Georgia, 2014[#]

15. **H. W. Hatch**, Y. Ding, J. Mittal and V. K. Shen, "Computational Study of Coarse-Grained Models for Monoclonal Antibodies" Gordon Research Conference: Water and Aqueous Solutions, Holderness School, Holderness, New Hampshire, 2014^{*}

14. **H. W. Hatch**, F. H. Stillinger and P. G. Debenedetti, "Thermodynamics and simulation of the negative pressure folding and unfolding of trp-cage and GB1 beta-hairpin miniproteins" American Institute of Chemical Engineers Annual Meeting, Hilton San Francisco Union Square, San Francisco, California, 2013[#]

13. **H. W. Hatch**, and P. G. Debenedetti, "Negative Pressure Folding and Unfolding Simulations of Trp-cage and GB1 Beta-hairpin Miniproteins" Gordon Research Conference: Chemistry and Physics of Liquids, Holderness School, Holderness, New Hampshire, 2013^{*}

12. **H. W. Hatch**, and P. G. Debenedetti, "Molecular Modeling of Mechanical Stresses on Proteins in Glassy Matrices" Gordon Research Conference: Water and Aqueous Solutions, Holderness School, Holderness, New Hampshire, 2012^{*}

11. **H. W. Hatch**, and P. G. Debenedetti, "Molecular Modeling of Mechanical Stresses on Proteins in Glassy Matrices" Gordon-Kenan Research Seminar: Water and Aqueous Solutions, Holderness School, Holderness, New Hampshire, 2012^{*}

10. **H. W. Hatch**, and P. G. Debenedetti, "Molecular Modeling of Mechanical Stresses on Proteins in Glassy Carbohydrate-Water Matrices" Chemical and Biological Engineering Graduate Student Symposium, Princeton University, Princeton, New Jersey, 2011[#]

9. **H. W. Hatch**, and P. G. Debenedetti, "Molecular Modeling of Mechanical Stresses on Proteins in Glassy Carbohydrate-Water Matrices" American Institute of Chemical Engineers Annual Meeting, Minneapolis Convention Center, Minneapolis, Minnesota, 2011[#]

8. **H. W. Hatch**, T. G. Lombardo, F. H. Stillinger and P. G. Debenedetti, "Microscopic Models of Chiral Amplification and Symmetry Breaking" American Institute of Chemical Engineers Annual Meeting, Salt Palace Convention Center, Salt Lake City, Utah, 2010[#]

7. **H. W. Hatch**, and P. G. Debenedetti, "Computational studies of Mechanical Stresses on Proteins in the Glassy State" American Institute of Chemical Engineers Annual Meeting, Salt Palace Convention Center, Salt Lake City, Utah, 2010[#]
6. **H. W. Hatch**, T. G. Lombardo, F. H. Stillinger and P. G. Debenedetti, "Microscopic Models of Chiral Amplification and Symmetry Breaking" Gordon Research Conference: Water and Aqueous Solutions, Holderness School, Holderness, New Hampshire, 2010*
5. **H. W. Hatch**, "Water-like Dynamic Anomalies in a Repulsive Spherical Model" Princeton Research Symposium, Princeton University, Princeton, New Jersey 2008*
4. **H. W. Hatch** and H. S. Ashbaugh, "Stability of Natively Unfolded Proteins" AIChE Southern Regional Conference, Auburn University, Auburn, Alabama 2008[#]
3. **H. W. Hatch** and P. Q. Clancy, "Simulation of Type I Methane Hydration using the Fluctuating Charge Model" Cornell Center for Materials Research Colloquium Paper, Cornell University, Ithaca, New York 2007[#]
2. **H. W. Hatch** and H. S. Ashbaugh, "Stability of Natively Unfolded Proteins" MGE@MSA/WAESO Research Conference, University of Arizona, Tucson, Arizona 2007*
1. **H. W. Hatch**, "Protein Phase Transitions" MGE@MSA/WAESO Research Conference, University of Arizona, Tucson, Arizona 2006*

Relevant Computer Skills

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

Simulation Packages: LAMMPS, GROMACS, VMD, AMBER

Software Engineering: Git revision control, Google unit test

- Customized LAMMPS: Local Stress Calculation and Enthalpy/Rigid Body Minimization
- Developed Custom Programs: WL-TMMC in grand canonical and expanded ensembles, MD, DMD, Lattice Kinetic MC

HPC Cluster Building and Administration: PUIAS Linux, Rocks, Windows Server

- Built and Administered PGD Group HPC Cluster (3.3+ million CPU hours utilized)
- Administered websites for PGD, PGD Group and hhatch.com

Other Software: Gnuplot, MATLAB, Mathematica, Office, Zotero, LaTeX

References

Prof. Pablo G. Debenedetti

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