

# Nathan A. Mahynski, Ph.D.

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Chemical Informatics Group  
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## PROFESSIONAL BACKGROUND

Director, NIST MML Summer Undergraduate Research Fellowship (SURF) Program	2021 – present
Research Chemical Engineer, Chemical Informatics Group, NIST	2017 – present
<ul style="list-style-type: none"><li>• Primary focus areas: computational self-assembly of soft matter systems, machine learning, food safety, molecular simulations and algorithms.</li></ul>	
NRC Postdoctoral Fellowship, NIST	2015 – 2017

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## EDUCATION

Ph.D. Chemical Engineering, certificate in Computational and Information Science Princeton University, Princeton, NJ	2015
M.A. Chemical Engineering Princeton University, Princeton, NJ	2012
B.S. Chemical Engineering, Minor in Chemistry Purdue University, West Lafayette, IN Magna Cum Laude	2010

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## SELECTED PROFESSIONAL AWARDS & HONORS

NIST MML Accolade	2020
<ul style="list-style-type: none"><li>• Citation: “For pioneering simulation work in colloidal self-assembly, adsorption science, and statistical-mechanical extrapolation algorithms”</li></ul>	
Named “Distinguished Young Scholar in Chemical Engineering” by Univ. of Washington	2016
Christopher J. Wormald Prize in Thermodynamics	2015
National Research Council (NRC) Research Associateship Program Fellowship, NIST	2015
Milliken Graduate Research Symposium Invited Speaker	2015
Gordon Wu Prize for Excellence, Princeton University	2014
National Science Foundation Young Researcher Award (FOMMS Conference)	2012
National Science Foundation Graduate Research Fellowship	2011

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## AFFILIATIONS

Sigma Xi Scientific Research Honor Society	2017–present
Tau Beta Pi Engineering Honor Society	2010–present
American Institute of Chemical Engineers (AIChE)	2007–present
American Physical Society (APS)	2019–present

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## PUBLISHED WORKS (h index = 14)

40. "Seabird Tissue Archival and Monitoring Project (STAMP) Data from 1999-2010," N. A. Mahynski, J. M. Ragland, S. S. Schurr, R. Pugh, V. K. Shen, *J. Res. NIST* **126**, 126028 (2021).  
Data published at: <https://doi.org/10.18434/mds2-2431> with analysis on github.
39. "Symmetry-derived structure directing agents for two-dimensional crystals of arbitrary colloids," N. A. Mahynski, V. K. Shen, *Soft Matter* **17**, 7853–7866 (2021).
38. "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, V. K. Shen, *J. Chem. Phys.* **153**, 144101 (2020).
37. "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, V. K. Shen, *Molecular Simulation* 1–13 (2020).  
Invited review article.
36. "Symmetry-based crystal structure enumeration in two dimensions," E. Pretti, V. K. Shen, J. Mittal, N. A. Mahynski, *J. Phys. Chem. A* **124**, 3276–3285 (2020).
35. "Grand canonical inverse design of multicomponent colloidal crystals," N. A. Mahynski, R. Mao, E. Pretti, V. K. Shen, J. Mittal, *Soft Matter* **16**, 3187–3194 (2020).  
Featured on the inside cover.
34. "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**, 1279–1286 (2020).
33. "Using symmetry to elucidate the importance of stoichiometry in colloidal crystal assembly," N. A. Mahynski, E. Pretti, V. K. Shen, J. Mittal, *Nature Commun.* **10**, 2028 (2019).  
"Behind the paper" summary, *Nature Chemistry Community Blog*, May 2019.
32. "On the virial coefficients of confined fluids: analytic expressions for the thermodynamic properties of hard particles with attractions in slit and cylindrical pores to second order," W. P. Krekelberg, N. A. Mahynski, V. K. Shen, *J. Chem. Phys.* **150**, 044704 (2019).
31. "Flat-histogram monte carlo as an efficient tool to evaluate adsorption processes involving rigid and deformable molecules," M. Witman, N. A. Mahynski, B. Smit, *J. Chem. Theory Comput.* **14**, 6149–6158 (2018).
30. "Monte carlo simulation of cylinders with short-range attractions," H. W. Hatch, N. A. Mahynski, R. P. Murphy, M. A. Blanco, V. K. Shen, *AIP Advances* **8**, 095210 (2018).
29. "Assembly of three-dimensional binary superlattices from multi-flavored particles," E. Pretti, H. Zerbe, M. Song, Y. Ding, N. A. Mahynski, H. W. Hatch, V. K. Shen, J. Mittal, *Soft Matter* **14**, 6303–6312 (2018).
28. "Predicting structural properties of fluids by thermodynamic extrapolation," N. A. Mahynski, S. Jiao,<sup>1</sup> H. W. Hatch, M. A. Blanco, V. K. Shen, *J. Chem. Phys.* **148**, 194105 (2018).  
Featured as an "Editor's Pick" article and "Scilight".
27. "Molecular simulation of capillary phase transitions in flexible porous materials," V. K. Shen, D. W. Siderius, N. A. Mahynski, *J. Chem. Phys.* **148**, 124115 (2018).
26. "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).
25. "Multivariable extrapolation of grand canonical free energy landscapes," N. A. Mahynski, J. R. Errington, V. K. Shen, *J. Chem. Phys.* **147**, 234111 (2017).
24. "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).
23. "Assembly of multi-flavored two-dimensional colloidal crystals," N. A. Mahynski, H. Zerbe, H. W. Hatch, V. K. Shen, J. Mittal, *Soft Matter* **13**, 5397–5408 (2017).
22. "Temperature extrapolation of multicomponent grand canonical free energy landscapes," N. A. Mahynski, J. R. Errington, V. K. Shen, *J. Chem. Phys.* **147**, 054105 (2017).

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<sup>1</sup>Contributions equal to first author

21. "Void-based assembly of colloidal crystals," N. A. Mahynski, L. Rovigatti, C. N. Likos, A. Z. Panagiotopoulos, *G.I.T. Laboratory Journal Europe* **21**, 32–34 (2017).
20. "Controlling relative polymorph stability in soft porous crystals with a barostat," N. A. Mahynski, V. K. Shen, *J. Chem. Phys.* **146**, 224706 (2017).
19. "Directionally interacting spheres and rods form ordered phases," W. Liu, N. A. Mahynski,<sup>2</sup> O. Gang, A. Z. Panagiotopoulos, S. K. Kumar, *ACS Nano* **11**, 4950–4959 (2017).
18. "Relationship between pore-size distribution and flexibility of adsorbent materials: Statistical mechanics and future material characterization techniques," D. W. Siderius, N. A. Mahynski, V. K. Shen, *Adsorption* **23**, 593–602 (2017).
17. "Predicting low-temperature free energy landscapes with flat-histogram monte carlo methods," N. A. Mahynski, M. A. Blanco, J. R. Errington, V. K. Shen, *J. Chem. Phys.* **146**, 074101 (2017).
16. "Reentrant equilibrium disordering in nanoparticle–polymer mixtures," D. Meng, S. K. Kumar, G. S. Grest, N. A. Mahynski, A. Z. Panagiotopoulos, *npj Computational Materials* **3**, 3 (2017).
15. "Tuning flexibility to control selectivity in soft porous crystals," N. A. Mahynski, V. K. Shen, *J. Chem. Phys.* **146**, 044706 (2017).
14. "Multicomponent adsorption in mesoporous flexible materials with flat-histogram monte carlo methods," N. A. Mahynski, V. K. Shen, *J. Chem. Phys.* **145**, 174709 (2016).
13. "Entropic control over nanoscale colloidal crystals," N. A. Mahynski, *Mol. Phys.* **114**, 2586–2596 (2016).
12. "Bottom-up with a twist: a new approach for colloidal crystal assembly," N. A. Mahynski, L. Rovigatti,<sup>3</sup> C. N. Likos, A. Z. Panagiotopoulos, *ACS Nano* **10**, 5459–5467 (2016).
11. "Coarse-graining and phase behavior of model star polymer–colloid mixtures in solvents of varying quality," A. Nikoubashman, N. A. Mahynski, B. Capone, A. Z. Panagiotopoulos, C. N. Likos, *J. Chem. Phys.* **143**, 243108 (2015).  
 Featured in Special Topic Issue: "Coarse Graining of Macromolecules, Biopolymers, and Membranes," *J. Chem. Phys.* **143**, 24 (2015).
10. "Tuning polymer architecture to manipulate the relative stability of different colloid crystal morphologies," N. A. Mahynski, S. K. Kumar, A. Z. Panagiotopoulos, *Soft Matter* **11**, 5146–5153 (2015).
9. "Grafted nanoparticles as soft patchy colloids: self-assembly versus phase separation," N. A. Mahynski, A. Z. Panagiotopoulos, *J. Chem. Phys.* **142**, 074901 (2015).
8. "Relative stability of the fcc and hcp polymorphs with interacting polymers," N. A. Mahynski, S. K. Kumar, A. Z. Panagiotopoulos, *Soft Matter* **11**, 280–289 (2015).
7. "Stabilizing colloidal crystals by leveraging void distributions," N. A. Mahynski, A. Z. Panagiotopoulos, D. Meng, S. K. Kumar, *Nature Commun.* **5**, 4472 (2014).  
 Featured article in *Photonics Spectra* Issue 10, Vol 48, p. 26, October 2014.  
 Featured in *Discovery: Research at Princeton* 2014–2015 Annual Issue, p. 5.
6. "Flow-induced demixing of polymer–colloid mixtures in microfluidic channels," A. Nikoubashman, N. A. Mahynski, A. Pirayandeh, A. Z. Panagiotopoulos, *J. Chem. Phys.* **140**, 094903 (2014).  
*J. Chem. Phys.* 2014 Editors' Choice in "Polymers and Soft Matter" Division.
5. "Phase behavior of athermal colloid–star polymer mixtures," N. A. Mahynski, A. Z. Panagiotopoulos, *J. Chem. Phys.* **139**, 024907 (2013).
4. "Structure of phase-separated athermal colloid–polymer systems in the protein limit," N. A. Mahynski, B. Irick, A. Z. Panagiotopoulos, *Phys. Rev. E* **87**, 022309 (2013).
3. "Pressure and density scaling for colloid–polymer systems in the protein limit," N. A. Mahynski, T. Lafitte, A. Z. Panagiotopoulos, *Phys. Rev. E* **85**, 051402 (2012).
2. "Reduced water density in a poly(ethylene oxide) brush," H. Lee, D. H. Kim, H.-W. Park, N. A. Mahynski, K. Kim, M. Meron, B. Lin, Y.-Y. Won, *J. Phys. Chem. Lett.* **3**, 1589–1595 (2012).

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<sup>2</sup>Contributions equal to first author

<sup>3</sup>Contributions equal to first author

1. "Crystallization of bidisperse repulsive colloids in two-dimensional space: a study of model systems constructed at the air-water interface," J. Hur, N. A. Mahynski, Y.-Y. Won, *Langmuir* **26**, 11737–11749 (2010).

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## PRESENTATIONS

Poster [†], Invited Talk [‡].

40. "Developing chemometric fingerprints to identify seabirds in the northern pacific," N. A. Mahynski, J. M. Ragland, S. S. Schurr, V. K. Shen, *Pacificchem: The International Chemical Congress of Pacific Basin Societies*, Honolulu, HI USA [virtual] (12/2021). [†]
39. "Self-Assembly templates for two-dimensional colloidal crystals derived from symmetry," N. A. Mahynski, V. K. Shen, *American Institute of Chemical Engineers Annual Meeting*, Boston, MA USA (11/2021).
38. "Development of a web-based repository of stable isotope and trace element measurements in food and related matrices," N. Blonder, N. A. Mahynski, V. K. Shen, *Research Coordination Meeting of CRP D52042 "Implementation of Nuclear Techniques for AuthenticCaTion of Foods with High-Value Labelling Claims" (INTACT Food)*, Virtual (11/2021).
37. "Symmetry-based discovery of multicomponent, two-dimensional colloidal crystals," N. A. Mahynski, E. Pretti, V. K. Shen, J. Mittal, *American Physical Society March Meeting*, Denver, CO USA [virtual] (03/2021).
36. "Symmetry-based discovery of multicomponent, two-dimensional colloidal crystals," N. A. Mahynski, E. Pretti, V. K. Shen, J. Mittal, *GRC: Colloidal, Macromolecular & Polyelectrolyte Solutions*, Ventura, CA USA (02/2020). [†]
35. "Grand canonical inverse design of multicomponent colloidal assemblies," N. A. Mahynski, E. Pretti, V. K. Shen, J. Mittal, *American Institute of Chemical Engineers Annual Meeting*, Orlando, FL USA (11/2019).
34. "Symmetry-based discovery of multicomponent, two-dimensional colloidal crystals," N. A. Mahynski, E. Pretti, V. K. Shen, J. Mittal, *93<sup>rd</sup> ACS Colloid and Surface Science Symposium*, Atlanta, GA USA (06/2019).
33. "Symmetry-based discovery of multicomponent, two-dimensional colloidal crystals," N. A. Mahynski, E. Pretti, V. K. Shen, J. Mittal, *NIST CSD Research Day*, Gaithersburg, MD USA (05/2019). [†]
32. "Symmetry-based discovery of multicomponent colloidal crystals," N. A. Mahynski, *Mid-Atlantic Soft Matter Workshop*, Institute for Bioscience and Biotechnology Research, Rockville, MD USA (02/2019).
31. "Symmetry-based discovery of multicomponent, two-dimensional colloidal crystals," N. A. Mahynski, E. Pretti, V. K. Shen, J. Mittal, *American Institute of Chemical Engineers Annual Meeting*, Pittsburgh, PA USA (11/2018).
30. "Symmetry-based discovery of multicomponent, two-dimensional colloidal crystals," N. A. Mahynski, E. Pretti, V. K. Shen, J. Mittal, *Foundations of Molecular Modeling and Simulation*, Delavan, WI USA (07/2018). [†]
29. "Predicting the free energy landscape of multicomponent fluids," N. A. Mahynski, J. R. Errington, V. K. Shen, *American Institute of Chemical Engineers Annual Meeting*, Minneapolis, MN USA (11/2017).
28. "Predicting the free energy landscape of multicomponent fluids," N. A. Mahynski, J. R. Errington, V. K. Shen, *Thermodynamics 2017*, Edinburgh, Scotland (09/2017).
27. "Self-assembly of multi-flavored two-dimensional binary colloidal crystals," N. A. Mahynski, H. Zerbe, H. W. Hatch, V. K. Shen, J. Mittal, *Thermodynamics 2017*, Edinburgh, Scotland (09/2017). [†]
26. "Self-assembly of multi-flavored two-dimensional binary colloidal crystals," N. A. Mahynski, H. Zerbe, H. W. Hatch, V. K. Shen, J. Mittal, *91<sup>st</sup> ACS Colloid and Surface Science Symposium*, New York, NY USA (07/2017).
25. "Characterizing multi-flavored assembly of two dimensional binary colloidal crystals," N. A. Mahynski, V. K. Shen, H. Zerbe, J. Mittal, *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA USA (11/2016).

24. "Polymer-mediated polymorphic control over open colloidal crystals," **N. A. Mahynski**, L. Rovigatti, C. N. Likos, A. Z. Panagiotopoulos, *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA USA (11/2016).
23. "Self-assembly of directionally interacting spheres and rods," **N. A. Mahynski**, W. Liu, O. Gang, A. Z. Panagiotopoulos, S. K. Kumar, *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA USA (11/2016).
22. "Effect of adsorbent material properties on the selective separation of supercritical multicomponent fluid mixtures," **N. A. Mahynski**, V. K. Shen, *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA USA (11/2016).
21. "Entropic control over nanoscale colloidal crystals," **N. A. Mahynski**, S. K. Kumar, A. Z. Panagiotopoulos, *American Institute of Chemical Engineers Annual Meeting*, San Francisco, CA USA (11/2016).
20. "Structure-directing soft matter agents: a new twist on colloidal crystal assembly," **N. A. Mahynski**, *Distinguished Young Scholars Seminar*, University of Washington, Seattle, WA USA (08/2016). [†]
19. "Structure-directing soft matter agents: a new twist on colloidal crystal assembly," **N. A. Mahynski**, *Condensed Matter Theory Seminar*, Johannes Gutenberg University am Mainz, Mainz Germany (06/2016). [†]
18. "Effects of adsorbent material properties on the selective separation of non-ideal multicomponent fluid mixtures," **N. A. Mahynski**, V. K. Shen, *8<sup>th</sup> International Conference on Porous Media Annual Meeting*, Cincinnati, OH USA (05/2016). [†]
17. "Effects of adsorbent material properties on the selective separation of non-ideal multicomponent fluid mixtures," **N. A. Mahynski**, V. K. Shen, *12<sup>th</sup> International Conference on the Fundamentals of Adsorption*, Graf-Zeppelin-Haus, Friedrichshafen/Lake Constance Germany (05/2016). [†]
16. "Entropic control over nanoscale colloidal crystals," **N. A. Mahynski**, S. K. Kumar, A. Z. Panagiotopoulos, *NIST Sigma Xi PPP*, Gaithersburg, MD (02/2016). [†]  
Sigma Xi Outstanding Poster Award, 2016
15. "Entropic control over nanoscale colloidal crystals," **N. A. Mahynski**, S. K. Kumar, A. Z. Panagiotopoulos, *GRC: Colloidal, Macromolecular & Polyelectrolyte Solutions*, Ventura, CA USA (02/2016). [†]
14. "Structure-directing soft matter agents: a new paradigm for colloidal assembly," **N. A. Mahynski**, *Mid-Atlantic Soft Matter Workshop*, National Institutes of Health, Bethesda, MD USA (01/2016).
13. "Entropic control over nanoscale colloidal crystals," **N. A. Mahynski**, S. K. Kumar, A. Z. Panagiotopoulos, *Thermodynamics*, Copenhagen, Denmark (09/2015). [†, plenary]
12. "Self-assembly of directionally interacting spheres and rods," **N. A. Mahynski**, W. Liu, O. Gang, A. Z. Panagiotopoulos, S. K. Kumar, *Thermodynamics*, Copenhagen, Denmark (09/2015). [†]
11. "Engineering entropy: polymorphic control over nanoscale colloidal crystals," **N. A. Mahynski**, S. K. Kumar, A. Z. Panagiotopoulos, *Brookhaven National Lab*, Upton, NY USA (04/2015). [†]
10. "Engineering entropy: polymorphic control over nanoscale colloidal crystals," **N. A. Mahynski**, S. K. Kumar, A. Z. Panagiotopoulos, *Milliken Graduate Research Symposium*, Spartanburg, SC USA (04/2015). [†]
9. "Engineering entropy: polymorphic control over colloidal crystals at the nanoscale," **N. A. Mahynski**, S. K. Kumar, A. Z. Panagiotopoulos, *National Institute of Standards and Technology*, Gaithersburg, MD USA (12/2014). [†]
8. "Polymer-grafted nanoparticles as patchy colloids," **N. A. Mahynski**, A. Z. Panagiotopoulos, *American Institute of Chemical Engineers Annual Meeting*, Atlanta, GA USA (11/2014).
7. "Stabilizing colloidal crystals by leveraging void distributions," **N. A. Mahynski**, A. Z. Panagiotopoulos, D. Meng, S. K. Kumar, *American Institute of Chemical Engineers Annual Meeting*, Atlanta, GA USA (11/2014).
6. "Stabilizing colloidal crystals by leveraging void distributions," **N. A. Mahynski**, A. Z. Panagiotopoulos, *Liquids 2014: 9th Liquid Matter Conference*, Lisbon, Portugal (07/2014). [†]
5. "Self-assembly and phase separation of nanoparticle amphiphiles," **N. A. Mahynski**, A. Z. Panagiotopoulos, *Liquids 2014: 9th Liquid Matter Conference*, Lisbon, Portugal (07/2014). [†]

4. "Polymer mediated colloidal crystal structure," **N. A. Mahynski**, A. Z. Panagiotopoulos, *Princeton Graduate Student Symposium*, Princeton, NJ USA (10/2013).
3. "Universality of depletion-induced phase behavior in colloid-star polymer systems," **N. A. Mahynski**, A. Z. Panagiotopoulos, *Thermodynamics*, Manchester, UK (09/2013).
2. "Phase behavior of colloid-polymer mixtures: density and pressure scaling," **N. A. Mahynski**, A. Z. Panagiotopoulos, *Princeton Graduate Student Symposium*, Princeton, NJ USA (10/2012). [†]
1. "Phase behavior of colloid-polymer mixtures: density and pressure scaling," **N. A. Mahynski**, A. Z. Panagiotopoulos, *Foundations of Molecular Modeling and Simulation*, Mt. Hood, OR USA (07/2012). [†]

## TEACHING AND PROFESSIONAL ENGAGEMENT

American Institute of Chemical Engineers

- Chair, "Recent Advances in Multiscale Methodologies" and "Thermodynamics at the Nanoscale" Sessions, 2021
- Chair, "Thermodynamics at the Nanoscale" Session, 2020
- Co-chair, "Thermodynamics at the Nanoscale" Session, 2019

NIST Summer Undergraduate Research Fellowship (SURF) Mentor

2016–present

National Institute of Standards and Technology

- Designed and supervised projects for undergraduate guest researchers concerning computational thermodynamics, statistical mechanics, and other computational self-assembly (simulation) problems.
- Daniel Markiewitz (Chemical Engineer, Cornell Univ. 2021), currently a graduate student at M.I.T.; Bliss Han (Environmental Engineering, Brown Univ. 2021).
- Kamryn Kant (Chemical Engineer, Clemson Univ. 2018).
- Evan Pretti (Chemical Engineer, Lehigh Univ. 2017), currently a graduate student at the University of California at Santa Barbara.
- Sally Jiao (Chemical Engineer, Princeton Univ. 2016, 2017), currently a graduate student at the University of California at Santa Barbara.

NSF Research Experience for Undergraduates (REU) Mentor

2012, 2013

Princeton University

- Mentored an undergraduate student each year in the art of scientific computing and molecular simulations pertaining to material science.
- These fruitful partnerships produced several papers published in peer-reviewed journals.

Assistant in Instruction, "Introduction to Thermodynamics"

2012

Princeton University, Department of Chemical & Biological Engineering

- Created and led biweekly review sessions emphasizing creative problem solving in thermodynamics. Responsible for grading and reviewing assignments, as well as weekly office hours. Assisted in editing and creating solution key for the course textbook, "Essential Thermodynamics," A. Z. Panagiotopoulos, Drios Press, 2011.
- Nominated by my students for the 2012 Princeton University Teaching award.

Teaching Assistant, "Honors Ordinary Differential Equations"

2008

Purdue University, Department of Mathematics

- Developed and taught weekly lectures on MatLab programming assignments to understand real-world phenomena like population models and elementary chaos.