

# Michael Grünwald

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## EDUCATION

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Ph.D. University of Vienna, Austria, 2009.  
Magister (M.Sc.) University of Vienna, Austria, 2005.

## PROFESSIONAL APPOINTMENTS

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since 01/2022 Assoc. Department Chair for Undergraduate Studies, University of Utah.  
since 07/2020 Associate Professor of Chemistry, University of Utah.  
08/2014 – 06/2020 Assistant Professor of Chemistry, University of Utah.  
11/2013 – 07/2014 University Assistant (Postdoctoral Researcher with Teaching Duties),  
Department of Physics, University of Vienna, Austria.  
11/2012 – 10/2013 Postdoctoral Researcher (Schrödinger Return Phase), Department of  
Physics, University of Vienna, Austria.  
08/2009 – 10/2012 Postdoctoral Researcher, Department of Chemistry, University of  
California, Berkeley. (Advisor: Phill Geissler)  
10/2004 – 07/2009 Graduate Student Researcher, Faculty of Physics, University of Vienna,  
Austria. (Advisor: Christoph Dellago)

## HONORS AND AWARDS

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2021 – 2022 UPSTEM Fellow  
2021 R. W. Parry Teaching Award  
2019 NSF Career Award  
2013 ASCINA Young Scientist Award  
2011 – 2013 Erwin Schrödinger Postdoctoral Fellowship

## Publications

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### UNIVERSITY OF UTAH

1. C. L. Bassani et al., Nanocrystal Assemblies: Current Advances and Open Problems, *Nanocrystal Assemblies: Current Advances and Open Problems*, ACS Nano 2024 (under review).
2. Y. Pimonova, J. E. Carpenter, and **M. Grünwald**, Thermodynamic Stability Is a Poor Indicator of Cocrystallization in Models of Organic Molecules, *Journal of the American Chemical Society* 2024 146 (4), 2805-2815, <https://doi.org/10.1021/jacs.3c13030>
3. Q. Wang, J. Rimsza, J. A. Harvey, P. Newell, **M. Grünwald**, and A. G. Ilgen, Molecular Dynamics Simulations of Calcite Fracture in Water, *The Journal of Physical Chemistry C* 2024 128 (1), 375-383, <https://doi.org/10.1021/acs.jpcc.3c05702>
4. Y. Eygeris, Q. Wang, M. Görke, **M. Grünwald**, and I. Zharov. Temperature-Responsive Nanoporous Membranes from Self-Assembly of Poly(N-isopropylacrylamide) Hairy Nanoparticles, *ACS Applied Materials & Interfaces* 2023 15 (24), 29384-29395, <https://doi.org/10.1021/acsmi.3c05072>
5. 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. Schneider, N. Schwierz, D.A. Sivak, S. Vaikuntanathan, S. Whitlam, A. Widmer-Cooper, Remembering the Work of Phillip L. Geissler: A Coda to His Scientific Trajectory, *Remembering the Work of Phillip L. Geissler: A Coda to His Scientific Trajectory*, *Annu. Rev. Phys. Chem.* (2022), DOI: <https://doi.org/10.1146/annurev-physchem-101422-030127>.
6. H. Zhu, Z. Fan, S. Song, D. Eggert, Y. Liu, W. Shi, Y. Yuan, K.-S. Kim, **M. Grünwald** & O. Chen, Dual Atomic Coherence in the Self-Assembly of Patchy Heterostructural Nanocrystals, *ACS Nano* (2022), 16, 9, 15053-15062, DOI: <https://doi.org/10.1021/acsnano.2c06167>.
7. J.E. Carpenter and **M. Grünwald**, Pre-Nucleation Clusters Predict Crystal Structures in Models of Chiral Molecules. *JACS* (2021), 143, 51, 21580-21593. DOI: <https://doi.org/10.1021/jacs.1c09321>.
8. Y. Nagaoka, M. Suda, I. Yoon, N. Chen, H. Yang, Y. Liu, B. Anzures, S. Parman, Z. Wang, **M. Grünwald**, H. M. Yamamoto, and O. Chen, Bulk Grain-Boundary Materials from Nanocrystals, *Chem* (2021), 7 (2), 509-525. <https://doi.org/10.1016/j.chempr.2020.12.026>
9. J.E. Carpenter and **M. Grünwald**, Heterogeneous Interactions Promote Crystallization and Spontaneous Resolution of Chiral Molecules. *JACS* (2020), 142 (24), 10755-10768. DOI: <https://doi.org/10.1021/jacs.0c02097>.
10. C.G. Bischak, M. Lai, D. Lu, Z. Fan, P. David, D. Dong, H. Chen, A.S. Etman, T. Lei, J. Sun, **M. Grünwald**, D. T. Limmer, P. Yang, and N. Ginsberg, Liquid-Like Interfaces Mediate Structural Phase Transitions in Lead Halide Perovskites. *Matter* 3 (2), 534-545, 2020. DOI: <https://doi.org/10.1016/j.matt.2020.07.015>.
11. Z. Fan and **M. Grünwald**, Energy vs. Entropy in Superlattices of Ligand-Covered Nanoparticles. Preprint: ChemRxiv (2019), <https://doi.org/10.26434/chemrxiv.9178037.v1>
12. H. Zhu, Z. Fan, L. Yu, M. A. Wilson, ..., **M. Grünwald**, and O. Chen, Controlling Nanoparticle Orientations in the Self-Assembly of Patchy Quantum Dot-Gold Heterostructural Nanocrystals, *JACS* (2019), 141 (14), pp 6013-6021, DOI:10.1021/jacs.9b01033.

13. Z. Fan and **M. Grünwald**, Orientational Order in Self-Assembled Nanocrystal Superlattices, *JACS* (2019), 141 (5), pp 1980-1988, DOI: 10.1021/jacs.8b10752.
14. Y. Eygeris, E. V. White, Q. Wang, J. E. Carpenter, **M. Grünwald**, and I. Zharov, Responsive nanoporous membranes with size selectivity and charge rejection from self-assembly of polyelectrolyte "hairy" nanoparticles, *ACS Appl. Mater. Interfaces*, 11, 3407 (2019), DOI: 10.1021/acsami.8b17483.
15. T. Schäfer, Z. Fan, **M. Grünwald**, and G. Kresse, Ab initio phase diagram of PbSe crystals calculated with the Random Phase Approximation, *Phys. Rev. B* 98, 144103 (2018).
16. H. Zhu, Z. Fan, Y. Yuan, M. A. Wilson, K. Hills-Kimball, Z. Wei, J. He, R. Li, **M. Grünwald**, and O. Chen. Self-Assembly of Quantum Dot-Gold Hetero-Dimer Nanocrystals with Orientational Order, *Nano Lett.* (2018), DOI: 10.1021/acs.nanolett.8b01860.
17. V. Nguyen and **M. Grünwald**, Microscopic origins of poor crystallinity in the synthesis of covalent-organic framework COF-5, *JACS* (2018), DOI: 10.1021/jacs.7b12529
18. L. Lupi, A. Hudait, B. Peters, **M. Grünwald**, R. G. Mullen, A. H. Nguyen, and V. Molinero, Role of Stacking Disorder in Ice Nucleation, *Nature* (2017), DOI: 10.1038/nature24279.
19. **M. Grünwald**, S. Tricard, G. M. Whitesides, and P. L. Geissler, Exploiting non-equilibrium phase separation for self-assembly, *Soft Matter* 12, 1517-1524 (2016), DOI: 10.1039/C5SM01922B

#### POSTDOCTORAL & GRADUATE

1. **M. Grünwald** and P. L. Geissler, Patterns without patches: Hierarchical assembly of complex structures from simple building blocks, *ACS Nano* 8, 5891 (2014).
2. H. Eshet, **M. Grünwald**, and E. Rabani, The electronic structure of CdSe/CdS core/shell seeded nanorods: type-I or quasi-type-II?, *Nano Letters* 13, 5880 (2013).
3. **M. Grünwald**, K. Lutker, A. P. Alivisatos, E. Rabani and P. L. Geissler, Metastability in pressure-induced structural transformations of CdSe/ZnS core/shell nanocrystals, *Nano Letters* 13, 1367 (2013).
4. **M. Grünwald**, A. Zayak, J. B. Neaton, P. L. Geissler, and E. Rabani, Transferable pair potentials for CdS and ZnS crystals, *J. Chem. Phys.* 136, 234111 (2012).
5. **M. Grünwald**, S. Jungblut, and C. Dellago, Transition path sampling of phase transitions: Nucleation and growth in materials hard and soft, in *Hierarchical Methods for Dynamics in Complex Molecular Systems*, IAS Series 10, Forschungszentrum Jülich (2012).
6. J. Henzie, **M. Grünwald**, A. Widmer-Cooper, P. L. Geissler, and P. Yang, Self-assembly of uniform polyhedral silver nanocrystals into densest packings and exotic superlattices, *Nature Materials* 11, 131 (2012).
7. **M. Grünwald** and C. Dellago, Transition path sampling studies of solid-solid transformations in nanocrystals under pressure, in "Trends in Computational Nanomechanics: Transcending Length and Time Scales" (Springer Series, 2010).
8. **M. Grünwald** and C. Dellago, Transition state analysis of solid-solid transformations in nanocrystals, *J. Chem. Phys.* 131, 164116 (2009).
9. **M. Grünwald** and C. Dellago, Nucleation and growth in structural transformations of nanocrystals, *Nano Letters* 9, 2099 (2009).
10. **M. Grünwald**, Phillip L. Geissler, and C. Dellago, Precision shooting: Sampling long transition pathways, *J. Chem. Phys.* 129, 194101 (2008).
11. **M. Grünwald**, Phillip L. Geissler, and C. Dellago, An efficient transition path sampling algorithm for nanoparticles under pressure, *J. Chem. Phys.* 127, 154718 (2007).

12. **M. Grünwald** and C. Dellago, Ideal gas pressure bath: a method for applying hydrostatic pressure in the computer simulation of nanoparticles, *Mol. Phys.* 104, 3709 (2006).
13. **M. Grünwald**, E. Rabani and C. Dellago, Mechanisms of the wurtzite to rocksalt transformation in CdSe nanocrystals, *Phys. Rev. Lett.* 96, 255701 (2006).

## Seminars & Presentations

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### INVITED SEMINARS & LECTURES

- 08/2023 Department of Chemistry, Washington University St. Louis.
- 07/2023 Institute of Science and Technology, Vienna, Austria.
- 06/2023 GRC Crystal Growth and Assembly 2023, Southern New Hampshire University.
- 04/2023 KITP Workshop: Nanoparticle Assemblies: A New Form of Matter with Classical Structure and Quantum Function, UC Santa Barbara, California.
- 02/2023 Department of Chemistry, University of Wisconsin, Madison.
- 12/2022 Statistical Thermodynamics & Molecular Simulations (STMS) Seminar Series.
- 09/2022 Keck Foundation Site Visit, University of Utah.
- 10/2021 Department of Chemistry, Dixie State University, Utah.
- 04/2020 FNANO 2020 (keynote), Snowbird, Utah.
- 12/2019 SM<sup>2</sup> Summer School 2019, University of Adelaide, Australia.
- 12/2019 Department of Chemistry, University of Sydney, Australia.
- 12/2019 Statistical Mechanics of Soft Matter 2019, University of Adelaide, Australia.
- 10/2019 Department of Chemistry, University of Colorado, Boulder.
- 08/2019 GRC Chemistry and Physics of Liquids 2019, Holderness, New Hampshire.
- 06/2019 Debye Colloquium, Debye Institute for Nano-Materials Science, Utrecht University, Netherlands.
- 06/2019 Seminar of the Chemical-Physical Society Vienna, University of Vienna, Austria.
- 05/2019 Department of Chemistry, University of Washington, Seattle, Washington.
- 04/2019 Department of Chemistry, Western Washington University, Washington.
- 03/2019 ACS National Meeting, Orlando, Florida.
- 01/2019 Berkeley Statistical Mechanics Meeting 2019, Berkeley, California.
- 12/2018 Statistical Mechanics of Soft Matter 2018, University of Auckland, New Zealand.
- 10/2018 Department of Chemistry, University of Chicago, Illinois.
- 09/2018 Department of Chemistry, Brown University, Providence, Rhode Island.
- 08/2018 Workshop "Entropy, Information and Order in Soft Matter", ICTS, Bangalore, India.
- 06/2018 Department of Chemistry, Braunschweig University of Technology, Braunschweig, Germany.
- 06/2018 CNRS, Sorbonne University, Paris, France.
- 06/2018 CECAM workshop "Multi-scale modeling of flexible and disordered porous materials", Paris, France.
- 02/2018 Foundry Seminar Series, Molecular Foundry, Lawrence Berkeley National Laboratory.
- 11/2017 Department of Chemistry, Whitworth University, Spokane, Washington.
- 11/2016 *Complex materials from self-assembly*, Department of Physics, University of Utah.
- 10/2016 *Complex materials from self-assembly*, Department of Material Science and Engineering, University of Utah.
- 09/2016 *Nucleation and growth in metal-organic frameworks*, CECAM workshop "Structure formation in soft colloids", Vienna University of Technology, Austria.
- 07/2016 *Self-assembly and structural transformations in nanomaterials – insights from computer simulation*, Department of Physics, University of Leoben, Austria.

- 07/2016 *Complex materials from self-assembly – insights from computer simulations*, Laboratoire de Physique et Chimie des Nano-Objets, INSA, CNRS, University of Toulouse, France.
- 06/2015 *Self-assembly of complex patterns from simple building blocks*, GRC Crystal Growth & Assembly, UNE Biddeford, Maine.
- 04/2015 *Complex patterns from simple rules*, Symposium in honor of Jack Simons, University of Utah, Salt Lake City.

#### CONTRIBUTED SEMINARS & PRESENTATIONS

- 12/2018 6th International Conference on Metal-Organic Frameworks & Open Framework Compounds (MOF2018), Auckland, New Zealand
- 03/2018 ACS National Meeting 2018, New Orleans, Louisiana.
- 01/2018 Berkeley Statistical Mechanics Meeting, UC Berkeley, California.
- 08/2017 *Molecular dynamics of porous framework formation*, Liquids GRC 2017, Holderness, New Hampshire.
- 05/2017 *Molecular dynamics of porous framework formation*, Self-assembly GRC 2017, Les Diablerets, Switzerland.
- 09/2016 *Molecular Dynamics of ZIF-8 Formation*, 5th International Conference on Metal-Organic Frameworks & Open Framework Compounds (MOF2016), Long Beach, California.
- 12/2015 *Exploiting non-equilibrium phase separation for self-assembly*, Pacificchem 2015, Honolulu, Hawaii.

#### SEMINARS & PRESENTATIONS BY STUDENTS/POSTDOCS

- 01/2020 J. Carpenter & M. Gruenwald, *Using Kinetics to Predict Crystal Structures*, Berkeley Statistical Mechanics Meeting 2020.
- 01/2020 N. Olsen & M. Gruenwald, *Using Kinetics to Predict Crystal Structures*, Berkeley Statistical Mechanics Meeting 2020.
- 08/2019 J. Carpenter & M. Gruenwald, *Revealing Mechanisms of Spontaneous Chiral Resolution with Molecular Models*, Liquids GRC 2019, Holderness, New Hampshire.
- 08/2019 C. Chu-Jon & M. Gruenwald, *Self-Assembly of tiny nanoparticles with thiol ligands*, GRC Chemistry and Physics of Liquids 2019, Holderness, New Hampshire.
- 05/2019 P. David & M. Gruenwald, *Neural-Network Representation of High-Dimensional Perovskite Potential Energy Surfaces*, RMACC Symposium 2019, Boulder, Colorado.
- 01/2019 Z. Fan & M. Gruenwald, *Self-assembly of Hetero-Nanocrystals*, Berkeley 2019 Statistical Mechanics Meeting, Berkeley, California.
- 01/2019 Q. Wang & M. Gruenwald, *Responsive Membranes from Self-Assembly of Polymer-Grafted Nanoparticles*, Berkeley 2019 Stat. Mech. Meeting, Berkeley, California.
- 01/2019 P. David & M. Gruenwald, *Neural Network Potentials for complex inorganic materials*, Berkeley 2019 Statistical Mechanics Meeting, Berkeley, California.
- 03/2018 Z. Fan & M. Gruenwald, *Ligand Interactions Determine Orientational Order in Self-Assembled Nanocrystal Superlattices*, APS March Meeting 2018, LA, California.
- 03/2018 J. Carpenter & M. Gruenwald, *Revealing Mechanisms of Spontaneous Chiral Resolution with Molecular Models*, APS March Meeting 2018, Los Angeles, California.
- 03/2018 V. Nguyen & M. Gruenwald, *Molecular Dynamics of Covalent Organic Framework Formation*, APS March Meeting 2018, Los Angeles, California.

- 03/2018 C. Chu-Jon & M. Gruenwald, *A Molecular Dynamics Model for ZIF-8 Formation*, APS March Meeting 2018, Los Angeles, California.
- 01/2018 Z. Fan & M. Gruenwald, *Understanding Nanocrystal Self-assembly Using Coarse-grained Simulations*, Berkeley 2018 Statistical Mechanics Meeting, Berkeley, California.
- 08/2017 M. Wilson & M. Gruenwald, *Self Assembly of Quantum Dot-Gold Satellite Nanocrystals*, University of Utah Undergraduate Research Summer Symposium.
- 08/2017 Z. Fan & M. Gruenwald, *Long-range and Short-range Orientational Order in Self-assembled Nanocrystal Superlattices*, GRC Chemistry and Physics of Liquids, Holderness, New Hampshire.
- 04/2017 D. Geisler & M. Gruenwald, *A framework for fitting atomistic energy landscapes with artificial neural networks*, University of Utah Undergraduate Research Symposium.
- 01/2017 V. Nguyen & M. Gruenwald, *Molecular Dynamics of COF-5 Formation*, Berkeley 2017 Statistical Mechanics Meeting, Berkeley, California.
- 01/2017 C. Chu-Jon & M. Gruenwald, *Molecular Dynamics of ZIF-8 Formation*, Berkeley 2017 Statistical Mechanics Meeting, Berkeley, California.
- 01/2017 Z. Fan & M. Gruenwald, *Pressure Induced B1-B33-B2 Phase Transitions in Lead Selenide*, Berkeley 2017 Statistical Mechanics Meeting, Berkeley, California.
- 09/2016 V. Nguyen & M. Gruenwald, *Molecular Dynamics of COF-5 Formation*, 5th International Conference on Metal-Organic Frameworks & Open Framework Compounds (MOF2016), Long Beach, California.
- 01/2016 E. Powell & M. Gruenwald, *Role of reversibility in the DNA-mediated self-assembly of colloids*, UC Berkeley 2016 Statistical Mechanics Meeting, Berkeley, California.
- 01/2016 C. Chu-Jon & M. Gruenwald, *Guiding Nucleation and Growth of Metal Organic Frameworks*, Berkeley 2016 Statistical Mechanics Meeting, Berkeley, California.
- 01/2016 P. David & M. Gruenwald, *Transformation Behavior and Structural Metastability of Nanoparticles under Shockwave Compression*, Berkeley 2016 Statistical Mechanics Meeting, Berkeley, California.
- 01/2016 N. Fox & M. Gruenwald, *Neural-Network Representation of High-Dimensional 2D Boron Potential-Energy Surfaces*, Berkeley 2016 Statistical Mechanics Meeting, California.

**INVITED (POSTDOCTORAL & GRADUATE)**

- 05/2014 *Structural metastability in nanocrystals under pressure*, DPG Spring Meeting, Dresden, Germany.
- 02/2013 *Thermodynamics and kinetics of self-assembly*, CECAM Winter School: Phase stability and phase transitions in soft and hard materials, St. Christoph, Austria.
- 10/2012 *Patterns without patches*, Statistical Mechanics Seminar Series, Berkeley, California.
- 09/2012 *Patterns without patches*, CECAM workshop "Design of self-assembling materials", Vienna.
- 01/2009 *Nucleation and growth in structural transformations of nanocrystals*, CompMat KickOff Symposium, TU Vienna.
- 11/2008 *Nucleation and growth in structural transformations of nanocrystals*, CMS Board Meeting 2008, TU Vienna.
- 02/2008 *Precision shooting: sampling diffusive transition pathways*, Workshop: Metastability and Rare Events in Complex Systems, Erwin Schrödinger Institute, Vienna.
- 09/2007 *Transition path sampling: Exploring rare events in complex systems*, Methods of Molecular Simulation 2007, Heidelberg, Germany.

01/2007 *Phase transformations in nanocrystals under pressure and binary symmetric fluid mixtures*, Conference on "Nucleation, Aggregation and Growth", Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India.

**CONTRIBUTED (POSTDOCTORAL & GRADUATE)**

02/2014 *Driving self-assembly with simple external forces*, ViCoM Conference: From electrons to phase transitions, Vienna.

09/2013 *Patterns without patches*, International Soft Matter Conference 2013, Rome, Italy.

05/2013 *Hierarchical self-assembly with simple interactions*, Gordon Research Seminar: Self-Assembly & Supramolecular Chemistry, Les Diablerets, Switzerland.

03/2011 *Directing the self-assembly of polyhedral silver nanocrystals*, APS Meeting 2011, Dallas.

01/2010 *Optimizing protocols of self-assembly*, Berkeley Mini Statistical Mechanics Meeting 2010, Transition Path Sampling Session, UC Berkeley, California.

09/2008 *Transition states in structural transformations of nanocrystals*, EMRS Fall Meeting 2008, Warsaw, Poland.



## Research Funding

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### CURRENT FUNDING

<u>Title of Project:</u>	"Predicting Kinetics of Molecular Crystallization Based on Solution Species"
Source:	Keck Foundation
Dates:	01/01/2023 – 12/31/2025
Co-PIs:	Michael Grünwald, Ryan Looper, Rodrigo Noriega
Amount:	\$1,000,000 (direct costs)
<u>Title of Project:</u>	"CAREER: Predicting nanocrystal superlattices based on ligand interactions"
Source:	NSF-DMR/CMMT
Dates:	04/01/2019 – 03/31/2024
PI:	Michael Grünwald
Amount:	\$500,000
<u>Title of Project:</u>	"REU Site: REU Site: Experimental and Computational Modeling of Materials and Biomolecular Systems"
Source:	NSF CHE
Dates:	05/15/2022 – 04/30/2025
Co-PIs:	Ming Hammond, Michael Grünwald
Amount:	\$364,500

### PAST FUNDING

<u>Title of Project:</u>	"Predicting the crystallization of chiral molecules "
Source:	NSF-CHE/CTMC
Dates:	06/01/2019 – 05/31/2023
PI:	Michael Grünwald
Amount:	\$450,000
<u>Title of Project:</u>	"REU Site: Catalysis in a Collaborative REU Program at the University of Utah"
Source:	NSF CHE
Dates:	09/01/2017 – 08/31/2022
Co-PIs:	Ming Hammond, Michael Grünwald
Amount:	\$330,000
<u>Title of Project:</u>	"Self-Assembly of Polymer-Brush Nanoparticles into Porous Supercrystals"
Source:	NSF CHE MSN & NSF DMR SSMC
Dates:	08/01/2017 – 07/31/2022
Co-PIs:	Ilya Zharov, Michael Grünwald
Amount:	\$462,911 (PI's portion: \$110,000)

Title of Project: "Guiding Nucleation and Growth of Metal-Organic Frameworks"  
Source: ACS Petroleum Research Fund  
Dates: 09/01/2016 – 08/31/2018  
PI: Michael Grünwald  
Amount: \$110,000

Title of Project: "Neural Network Potentials for the Study of Semiconductor Nanocrystals."  
Source: University of Utah Funding Incentive Seed Grant  
Dates: 01/2015 – 12/2015  
PI: Michael Grünwald  
Amount: \$29,498

## Teaching

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Fall 2022 & Fall 23	CHEM 1220 General Chemistry II
Spring 2015-2022	CHEM 3070 Physical Chemistry II
Spring 2021	CHEM 7530 Molecular Simulations
Fall 2014 & Fall 2016	CHEM 7050 Classical Thermodynamics
Fall 2017, 2019, 2023	CHEM 7040 Statistical Thermodynamics

## Mentorship

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<u>Postdoc:</u>	Carol Pacheco, Rashed Hasan.
<u>Former Postdocs:</u>	John Carpenter, Vu Nguyen, Zhaochuan Fan (now at Suzhou Institute of Nano-tech and Nano-bionics).
<u>Current PhD Students:</u>	Yulia Pimonova, Will Matthews, Jon Aronoff.
<u>Graduated (Ph.D.):</u>	Carlos Chu-Jon (2022), Qiaoyi Wang (2022), Vu Nguyen (2020), John Carpenter (2021).
<u>Graduated (M.Sc.):</u>	Michael Goytia (2017), Luka Drca (2017), Nathan Fox (2018).
<u>Undergraduate researchers (past):</u>	Zachary Croasmun-Adams Nicholas Olsen (UROP 2019, now Columbia graduate school) Philippe David (UROP 2016, REU 2018, Goldwater Scholarship, now at Google) Mitchell Wilson (REU 2017, UROP 2018, BS Chemistry 2018, now at Myriad Genetics) Simone Longo (BS/MS Chemistry 2019, now PhD program U of U) Spencer Cadet (BS Chemistry 2018, now Louisiana medical school) Dietrich Geisler (BS Chemistry, Honors Thesis 2017, now at Cornell graduate school) Ryan Boschert (BS Chemistry 2015, now at ARUP Laboratories) Ethan Powell (REU 2015, now DPT program U of U)

## Service & Outreach

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### PROFESSIONAL SERVICE

Conference activities:	APS Meeting March 2018: focus topic organizer, Liquids GRC 2017: discussion leader
Journal Review:	JACS, Nat. Mater., Nano Lett., Nat. Comm., J. Chem. Phys., Acc. Chem. Res., ACS Nano, Langmuir, Chem. Mater., J. Phys. Chem., J. Chem. Theory Comput.
Grant Review:	NSF panel and ad-hoc reviewer (CHE, DMR), ACS-PRF proposal reviewer

### DEPARTMENTAL SERVICE

since 2022	Associate Chair of Undergraduate Studies
since 2022	Utah Chemistry Major Committee

2019-2022	Chair of Graduate Admissions
since 2019	Co-director, Chemistry REU
since 2017	Director, Braunschweig exchange program
2014 – 2021	Graduate Education Committee
2019	Undergraduate Education Committee
2018 – 2019	TEP Faculty Search Committee

#### UNIVERSITY SERVICE

since 2022	College of Science Curriculum Committee
since 2020	College of Science Council
since 2017	UROF proposal reviewer
since 2015	Seed Grant reviewer
2014 – 2019	CHPC User Council

#### OTHER ACTIVITIES

2021/2022	UPSTEM fellow
since 2018	Director, Learning Abroad program "Chemistry Research in Germany"

#### SYNERGISTIC ACTIVITIES & OUTREACH (EXAMPLES)

1. **Organized and directed undergraduate exchange program** with the Department of Chemistry, Braunschweig University of Technology, Germany. In this program, which is supported by the Office of Learning Abroad and the College of Science at Utah, 5-7 undergraduate Chemistry students from the University of Utah join research groups at Braunschweig each year for 12 weeks of summer research.
2. **Co-organized focus topic "Self-assembly of nano-structured, macromolecular, and nanoporous materials"** at the APS March meeting 2018. This focus topic (with a total of 5 sessions) brought together leading researchers from chemistry, physics, and material science to discuss current developments in self-assembly.
3. **Lead computational chemistry workshops for high school students** at the "Science Day at the U". As part of the outreach program of the University of Utah, the mission of "Science Day" is to attract future college students to STEM disciplines by showcasing cutting-edge research in hands-on workshops. In these workshops, the PI makes use of online simulation programs that allow students to discover the power of molecular dynamics computer simulations.
4. **Gave a "Science Night Live" research presentation** at a downtown Salt Lake City pub. Science Night Live is part of the outreach program of the College of Science of the University of Utah. These monthly presentations by College of Science faculty engage a diverse crowd consisting of University staff and the general public in a casual pub environment.
5. **Lead chemistry workshops ("A mole of marshmallows") at pre- and elementary schools** in Salt Lake City. It is one of the PI's priorities to spark the joy of discovery in young children. In these workshops, the PI combines the powerful visuals of computer simulations with hands-on experiments.