Curriculum Vitae

Christopher Knight, Computational Science/Team Lead
Argonne National Laboratory

Work Address

Computational Science Division
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Appointments

Position	*Institution (Supervisor)*	*Dates*
UChicago CASE Senior Scientist At-Large	University of Chicago	9/2022 - present
Computational Science/Team Lead	Argonne CPS (Timothy Williams)	5/2018 - present
Assistant Computational Scientist	Argonne CPS (Nichols Romero)	3/2018 - 5/2018
Assistant Computational Scientist	Argonne LCF (Nichols Romero)	9/2013 - 3/2018

Postdoctoral Appointments

Institution	*Supervisor*	*Dates*
Argonne National Laboratory	Gregory A. Voth	4/2010 - 9/2013
University of Chicago	Gregory A. Voth	4/2010 - 10/2010
University of Utah	Gregory A. Voth	4/2009 - 3/2010

Education

Institution (Preceptor)	*Degree*	*Date*	*Field*
The Ohio State University (Sherwin J. Singer)	Ph.D.	2009	Chemistry
Eastern Michigan University	B.S. w/ Honors	2003	Chemistry

Honors

Impact Argonne Award for Program Development Activities	2022
Impact Argonne Team Award for successful acceptance of Polaris	2022
Impact Argonne Team Award in support of the IPR of ALCF-3	2020
Argonne's Strategic Laboratory Leadership Program	2018
ANL Pacesetter Award - "Testing early versions of Intel KNL chip"	2017
ANL Computational Postdoctoral Fellowship	2011-2012
Ohio State University Presidential Fellowship	2008-2009
Undergraduate Honors Senior Thesis/Project and Symposium	2003
ACS Organic Chemistry Achievement Award	2002
Honors Undergraduate Fellowship	2002
Maurice Decoster Chemistry Scholarship	2002

Professional Societies and Activities

Member of the American Chemical Society (2003 - present)
Member of the Electrochemical Society (2012 - 2017)

Refereed for *15* scientific journals: AIP Advances, Chemical Physics Letters, Diamond and Related Materials, Energies, International Journal of Electrical and Computer Engineering, International Journal of High Performance Computing Applications, Journal of Chemical Physics, Journal of Chemical Theory and Computation, Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Macromolecules, Materials, Molecular Physics, Molecules, and Science.

Synergistic Activities

- ALCF Lead for Applications Integration on Aurora for the Exascale Computing Project (ECP) to ensure application teams are properly prepared for the Aurora exascale architecture (2021 - present)

Research Interests

- High-performance scientific computing & performance projections
- Statistical mechanics
- Computer simulations via first principle methods (Kohn-Sham and Orbital-Free DFT)
- Condensed phase simulations: classical and quantum dynamics, multiscale processes, accurate and computationally efficient simulation of chemical reactions
- Chemistry at interfaces: aqueous systems, batteries and supercapacitors (electrolyte/electrode), fuel cells (proton and hydroxide conductance), biofuels (carboxysome), and smart materials (self-healing, piezoelectric, magnetostrictive), nanoporous materials
- Interactions of matter with soft and hard X-ray pulses

Teaching & Work Experience

CPS: Chris is currently team lead for Chemistry and Materials Science in the Argonne Leadership Computing Facility (ALCF) and the recently established Computational Science Division (CPS) at Argonne. In CPS, Chris helps to develop new cross-cutting collaborations involving others in CPS and the computing divisions, across Argonne, and other institutions to help address some of the most challenging scientific problems through advanced computing and simulation. One focus of these efforts today is helping teams prepare for the Aurora exascale system supported by the BES Computational Chemical Sciences program.

ALCF Catalyst: As a member of the ALCF Catalyst team, Chris works closely with researchers to help them accomplish their scientific goals using leadership computational resources. Chris assists researchers with profiling and debugging their codes, provides general guidance on code parallelization, I/O, load-balancing, workflow design, and data management, and discusses strategies to prepare for future architectures. Important components of this work include training users on high-performance computing topics and collaborating with researchers to advance their scientific mission.

Guest Lectures at Harvard University: In Nov. 2015, Chris organized and presented lectures and a hands-on lesson in large-scale scientific computing as part of a course titled "APCOMP 290R - Extreme Computing: Project-based High Performance Distributed and Parallel Systems" at Harvard University with Sadasivan Shankar, Pavlos Protopapas, and Efthimios Kaxiras. Chris led six sessions, which included running jobs on Mira at ALCF, to educate how supercomputers can be used to address real-world problems, such as designing better batteries using kinetic Monte Carlo.

Mentored undergraduate and high school students: Center for Multiscale Theory and Simulation, University of Chicago (6/12-7/12)

Teaching Assistant: Department of Chemistry, The Ohio State University (9/03-9/04, 9/05-9/06)

Publications: 2157 citations; h-index 24; i10-index 34 (February 2023)

1. Victor Naden Robinson, Raja Ghosh, Colin K. Egan, Marc Riera, Christopher Knight, Francesco Paesani, and Ali Hassanali, "The behavior of methane-water mixtures under elevated pressures from simulations using many-body potentials" *J. Chem. Phys.* **156**, 194504 (2022)

2. Phay J. Ho, Christopher Knight, and Linda Young, "High-resolution and Elemental Contrast Fluorescence Imaging with Intense X-ray Pulses" *Structual Dynamics* **8**, 044101 (2021) (Editor's Pick; Cover Image).

3. Maria Carolina Muniz, Thomas E. Gartner III, Marc Riera, Christopher Knight, Shuwen Yue, Francesco Paesani, and Athanassios Z. Panagiotopoulos, "Vapor-liquid equilibrium of water with the MB-pol many-body potential" *J. Chem. Phys* **154**, 211103 (2021) (Editor's Pick).

4. Steven J. Plimpton and Christopher Knight, "Rendezvous algorithms for large-scale modeling and simulation" *J. Parallel Distr. Com.* **147**:184 (2021).

5. Phay J. Ho, Christopher Knight, and Linda Young, "Extended X-ray Emission Times of Clusters in Intense X-ray Pulses" *Phys. Rev. A* **101**:043413 (2020).

6. Phay J. Ho, Benedikt J. Daurer, Max F. Hantke, Johan Bielecki, Andre Al Haddad, Max Bucher, Gilles Doumy, Ken Ferguson, Tais Gorkhover, Christopher Knight, Stefan Moeller, Timur Osipov,

Dipanwita Ray, Steve Southworth, Anatoli Ulmer Peter Walter, Janos Hajdu, Linda Young, Filipe R.N.C. Maia, and Christoph Bostedt, "The role of transient resonances for ultra-fast imaging of organic samples" *Nat. Commun.* **11**:167 (2020).

7. Ahren Jasper, Lawrence Harding, Christopher Knight, and Yuri Georgievskii, "Anharmonic Rovibrational Partition Functions at High Temperatures: Tests of Reduced-Dimensional Models for Systems with up to Three Fluxional Modes" *J. Phys. Chem. A* **123**:6210 (2019).

8. Hasan Metin Aktulga, Chris Knight, Paul Coffman, Kurt A. O'Hearn, Tzu-Ray Shan, and Wei Jiang, "Optimizing the Performance of Reactive Molecular Dynamics Simulations for Multi-core Architectures", *IJHPCA* **33**:304 (2019)

9. Evgenii O. Fetisov, Mansi S. Shah, Christopher Knight, Michael Tsapatsis, and J. Ilja Siepmann, "Understanding the Reactive Adsorption of H2S and CO2 in Sodium-Exchanged Zeolites", *ChemPhysChem* **14**:512 (2018).

10. Daniel R. Moberg, Shelby C. Straight, Christopher Knight, and Francesco Paesani, "Molecular Origin of the Vibrational Structure of Ice Ih", *J. Phys. Chem. Lett.* **8**:2579 (2017)

11. Phay Ho and Chris Knight, "Large-scale Atomistic Calculations of Clusters in Intense X-ray Pulses", *J. Phys. B: At. Mol. Opt. Phys.* **50**:104003 (2017)

12. C. Huy Pham, Sandeep K. Reddy, Karl Chen, Chris Knight, and Francesco Paesani, "Many-Body Interactions in Ice", *J. Chem. Theory Comput.*, **13**:1778-1784 (2017)

13. Andrew D. White, Chris Knight, Glen M. Hocky, and Gregory A. Voth, "Improved Ab Initio Molecular Dynamics by Minimally Biasing with Experimental Data", *J. Chem. Phys.*, **146**:041102 (2017)

14. Phay J. Ho, Chris Knight, Miklos Tegze, Gyula Faigel, C. Bostedt, and Linda Young, "Atomistic three-dimensional coherent x-ray imaging of nonbiological Systems", *Phys. Rev. A*, **94**:063823 (2016).

15. Sandeep K. Reddy, Shelby C. Straight, Pushp Bajaj, C. Huy Pham, Marc Riera, Daniel R. Moberg, Miguel A. Morales, Chris Knight, Andreas W. Götz, and Francesco Paesani, "On the accuracy of the MB-pol many-body potential for water. I. Interaction energies, vibrational frequencies, and classical thermodynamic and dynamical properties from clusters to liquid water and ice", *J. Chem. Phys.*, **145**:194504 (2016) (2016 JCP Editor's Choice)

16. Evgenii O. Fetisov, I-F. Will Kuo, Chris Knight, Joost VandeVondele, Troy Van Voorhis, and J. Ilja Siepmann, "First Principles Monte Carlo Simulations of Reaction Equilibria in Compressed Vapors", *ACS Cent. Sci.*, **2**(6):409-415 (2016)

17. Chen Chen, Ying-Lung Steve Tse, Gerrick E. Lindberg, Chris Knight, and Gregory A. Voth, "Hydroxide Solvation and Transport in Anion Exchange Membranes", *J. Am. Chem. Soc.*, **138**(3):991-1000 (2016)

18. Revati Kumar, Chris Knight, Collin D. Wick, and Bin Chen, "Bringing Reactivity to the Aggregation-Volume-Bias Monte Carlo Based Simulation Framework: Water Nucleation Induced by a Reactive Proton", *J. Phys. Chem. B*, **119**(29):9068-9075 (2015)

19. Peng Bai, Mi Yeong Jeon, Limin Ren, Chris Knight, Michael W. Deem, Michael Tsapatsis, and J. Ilja Siepmann, "Discovery of optimal zeolites for challenging separations and chemical transformations using predictive materials modeling", *Nat. Commun.*, **6**:5912 (2015)

20. Ying-Lung Steve Tse, Chris Knight, and Gregory A. Voth, "An Analysis of Hydrated Proton Diffusion in Ab Initio Molecular Dynamics", *J. Chem. Phys.*, **142**:014104 (2015)

21. Alistar Ottochian, Guilhem Dezanneau, Clement Gilles, Paolo Raiteri, Chris Knight, and Julian D. Gale, "Influence of isotropic and biaxial strain on proton conduction in Y-doped $BaZrO_3$: a reactive molecular dynamics study", *J. Mat. Chem. A*, **2**(9):3127-3133 (2014).

22. Revati Kumar, Chris Knight, and Gregory A. Voth, "Exploring the Behavior of the Hydrated Excess Proton at Hydrophobic Interfaces", *Farad. Discuss.*, **167**:263-278 (2013)

23. Takefumi Yamashita, Yuxing Peng, Chris Knight, and Gregory A. Voth, "Computationally Efficient Multiconfigurational Reactive Molecular Dynamics", *J. Chem. Theory Comput.*, **8**(12):4863-4875 (2012) (Berny Schlegel Festschrift)

24. Chris Knight, Gerrick E. Lindberg, and Gregory A. Voth, "Multiscale Reactive Molecular Dynamics", *J. Chem. Phys.*, **137**(22):22A525 (2012) (Nonadiabatic Dynamics special issue)

25. Chris Knight and Gregory A. Voth, "Coarse-graining Away Electronic Structure: A Rigorous Route to Accurate Condensed Phase Interaction Potentials", *Mol. Phys.*, **110**(9-10):935-944 (2012) (Bill Miller special issue).

26. Chris Knight and Gregory A. Voth, "The Curious Case of the Hydrated Proton", *Acc. Chem. Res.*, **45**(1):101-109 (2012) (Water in Chemistry special issue).

27. Sherwin J. Singer and Chris Knight, "Hydrogen bond topology and proton ordering in ice and water clusters", *Adv. Chem. Phys.*, **147**:1 (2012).

28. Hui Zhang, Ali A. Hassanali, Yun Kyung Shin, Chris Knight, and Sherwin J. Singer, "The water-amorphous silica interface: Analysis of the Stern layer and surface conduction", *J. Chem. Phys.*, **134**(2):024705 (2011).

29. Ali Hassanali, Hui Zhang, Chris Knight, Yun Kyung Shin, and Sherwin J. Singer, "The dissociated amorphous silica surface: Model development and evaluation", *J. Chem. Theory Comput.*, **6** (11):3456 (2010).

30. Chris Knight, C. Mark Maupin, Sergei Izvekov, and Gregory A. Voth, "Defining condensed phase reactive force fields from *ab initio* molecular dynamics simulations: The case of the hydrated excess proton", *J. Chem. Theory Comput.*, **6**(10):3223 (2010).

31. Chris Knight and Sherwin J. Singer, "Site disorder in ice VII arising from hydrogen bond fluctuations", *J. Phys. Chem. A*, **113**(45):12433 (2009) (Russell Pitzer Festschrift).

32. Chris Knight and Sherwin J. Singer, "Hydrogen bond ordering in ice V and the transition to ice XIII", *J. Chem. Phys.*, **129**(16):164513 (2008).

33. Chris Knight and Sherwin J. Singer, "A re-examination of the ice III/IX hydrogen bond ordering phase transition ", *J. Chem. Phys.*, **125**(6):064506 (2006).

34. Chris Knight, Sherwin J. Singer, Jer-Lai Kuo, Tomas K. Hirsch, Lars Ojamäe and Michael L. Klein, "Hydrogen bond topology and the ice VII/VIII and Ih/XI proton ordering phase transitions", *Phys. Rev. E*, **73**(5):056113 (2006).

35. Chris Knight and Sherwin J. Singer, "Prediction of a phase transition to a hydrogen bond ordered form of ice VI", *J. Phys. Chem. B*, **109**(44):21040 (2005).

36. Sherwin J. Singer, Jer-Lai Kuo, Tomas K. Hirsch, Chris Knight, Lars Ojamäe and Michael L. Klein, "Hydrogen bond topology and the ice VII/VIII and Ih/XI proton ordering phase transitions", *Phys. Rev. Lett.*, **94**(13):135701 (2005).

37. Christopher Knight and M. C. Milletti, "Theoretical characterization of two reaction pathways for the intramolecular cyclization of 2-(3-benzylaminopropanoyl-amino)benzamide", *J. Mol. Struct.: THEOCHEM*, **724**:143 (2005).

Conference Publications

1. JaeHyuk Kwack, John Tramm, Colleen Bertoni, Yasaman Ghadar, Brian Homerding, Esteban Rangel, Christopher Knight, and Scott Parker, "Evaluation of Performance Portability of Applications and Mini-Apps across AMD, Intel, and NVIDIA GPUs" In P3HPC workshop, SC21, November 2021.

2. Sudheer Chunduri, Elise Jennings, Kevin Harms, Christopher Knight, and Scott Parker, "A generalized statistics-based model for predicting network-induced variability" In 10th International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems (PMBS'19), SC19, November 2019.

3. JaeHyuk Kwack, Thomas Applencourt, Colleen Bertoni, Yasaman Ghadar, Huihuo Zheng, Christopher Knight, and Scott Parker, "Roofline-based Performance Efficiency of HPC Benchmarks and Applications on Current Generation of Processor Architectures" 2019 Cray User Group (CUG) Meeting, May 2019, Montreal, Canada.

4. Preeti Malakar, Christopher Knight, Todd Munson, Venkatram Vishwanath, and Michael E. Papka, "Topology-aware Space-shared Co-analysis of Large-scale Molecular Dynamics Simulations" In Proceedings of the International Conference for High Performance Computing, Network, Storage and Analysis (SC'18), November 2018, Dallas, TX, USA.

5. Preeti Malakar, Christopher Knight, Todd Munson, Venkatram Vishwanath, and Michael E. Papka, "Scalable In situ Analysis of Molecular Dynamics Simulations" ISAV 2017, November 2017, Denver, CO, USA.

6. Huihuo Zheng, Christopher Knight, Giulia Galli, Marco Govoni, and Francois Gygi, "Performance optimization of WEST and Qbox on Intel Knights Landing" Intel Xeon Phi Users Group (IXPUG) Fall 2017, September 2017, Austin, TX, USA.

7. Scott Parker, Vitali Morozov, Sudheer Chunduri, Kevin Harms, Chris Knight, and Kalyan Kumaran, "Early Evaluation of the Cray XC40 Xeon Phi System 'Theta' at Argonne" Cray User Group (CUG) 2017, May 2017, Redmond, WA, USA.

8. Preeti Malakar, Venkatram Vishwanath, Christopher Knight, Todd Munson, and Michael Papka, "Optimal Execution of Co-analysis for Large-scale Molecular Dynamics Simulations" In Proceedings of the International Conference for High Performance Computing, Network, Storage and Analysis (SC'16), November 2016, Salt Lake City, Utah, USA.

9. Preeti Malakar, Venkatram Vishwanath, Todd Munson, Christopher Knight, Mark Hereld, Sven Leyffer, and Michael Papka, "Optimal scheduling of in-situ analysis for large-scale scientific simulations" In Proceedings of the International Conference for High Performance Computing, Network, Storage and Analysis (SC'15), November 2015, Austin, Texas, USA.

10. Nayong Kim, Richard Platania, Tom Keyes, Wei Huang, Chris Knight, Seun-jong Park, and Joohyun Kim, "Enabling Large-scale Biomolecular Conformation Search with Replica Exchange Statistical Temperature Molecular Dynamics (RESTMD) over HPC and Cloud Computing Resources" in *IEEE 29th International Conference on Advanced Information Networking and Applications Workshops (WAINA)*, 61-66 (2015).

11. Andrew M. Herring, Melissa A. Vandiver, Asley M. Maes, Himashu Sarode, E. Bryan Coughlin, Daniel M. Knauss, Yushan Yan, Gerrick E. Lindberg, Christopher Knight, Gregory A. Voth, Daniel Herbst, Thomas A. Witten, and Matthew W. Liberatore, "Fundamental Studies of Alkaline Exchange Membranes Towards Optimization in a Fuel Cell Environment", *ECS Trans.,* **50**(2): 2059-2066 (2012).

12. Gerrick E. Lindberg, Chris Knight, Lisa E. Feldberg, and Gregory A. Voth, "Molecular Dynamics Simulations of Hydroxide Solvation and Transport in Anionic Exchange Membranes", *ECS Trans.,* **50**(2): 2053-2058 (2012).

13. Yuxing Peng, Chris Knight, Philip Blood, Lonnie Crosby, Gregory A. Voth, "Extending Parallel Scalability of LAMMPS and Multiscale Reactive Molecular Simulations", XSEDE12, **37**:1-7 (ACM, New York, 2012).

14. Gerrick E. Lindberg, Chris Knight, Ryan Jorn, James F. Dama, and Gregory A. Voth, "Multiscale Simulation of Hydroxide Solvation and Transport in Anion Exchange Membranes", *ECS Trans.,* **41**(1):1785 (2011).

15. Himanshu Sarode, Melissa A. Vandiver, Ashley M. Maes, Benjamin Caire, James L. Horan, Yating Tan, Yifan Li, Gerrick E. Lindberg, James F. Dama, Chris Knight, Ryan Jorn, Martin E. Lenz, Robert Kasper, Shuang Gu, Bingzi Zhang, Sönke Seifert, Tsung-han Tsai, Wen X. Zhang, E. Bryan Coughlin, Daniel M. Knauss, Yushan Yan, Gregory A. Voth, Thomas A. Witten, Matthew W. Liberatore, and Andrew M. Herring, "Designing Alkaline Exchange Membranes from Scratch", *ECS Trans.,* **41**(1):1761 (2011).

16. Chris Knight and Sherwin J. Singer, "Theoretical study of a hydroxide ion within the ice-Ih lattice", *Physics and Chemistry of Ice* (Proceedings of the 11th International Conference on the Physics and Chemistry of Ice), ed., Werner F. Kuhs (Royal Soc. of Chemistry, 2007), p.339.

17. Chris Knight and Sherwin J. Singer, "Tackling the problem of hydrogen bond order and disorder", *Physics and Chemistry of Ice* (Proceedings of the 11th International Conference on the Physics and Chemistry of Ice), ed., Werner F. Kuhs (Royal Soc. of Chemistry, 2007), p.329.

Technical Reports

1. Huihuo Zheng, Christopher J. Knight, Marco Govoni, Giulia Galli, and Francois Gygi, "First-Principles Simulations of Functional Materials for Energy Conversion", (*Technical Report for the ALCF Theta Early Science Program*), Argonne National Laboratory, 2017.

2. Adrian W. Lange, Gard Nelson, Christopher Knight, and Gregory A. Voth, "Multiscale Molecular Simulations at the Petascale (Parallelization of Reactive Force Field Model for Blue Gene/Q)", (*ALCF-2 Early Science Program Technical Report*), Argonne National Laboratory, 2013.

Book Chapters

1. Preeti Malakar, Venkatram Vishwanath, Christopher Knight, Todd Munson, and Michael E. Papka (2022).. *Resource-Aware Optimal Scheduling of In Situ Analysis* In Hank Childs, Janine C. Bennet, and Christoph Garth (Eds.), In Situ Visualization for Computational Science (pp. 183-). Switzerland: Springer

2. Mark R. Fahey et. al., (2019). Theta and Mira at Argonne National Laboratory. In Jeffrey S. Vetter (Ed.), *Contemporary High Performance Computing: From Petascale toward Exascale, Volume 3* (pp. 31-59). Boca Raton, FL: CRC Press

Presentations

1. "Opportunities with Preparing Scientific Codes for Exascale", talk presented in session "Open-source Software in Chemistry" at Fall ACS 2022 meeting in Chicago, IL, Aug. 21-25, 2022.

2. "Opportunities With Preparing Scientific Codes for GPUs", Keynote talk presented at NVIDIA Day "Accelerating Research with GPUs" at University of Illinois Chicago, April 20, 2022.

3. "Performance Tuning with the Roofline Model on GPUs and CPUs", Talk presented by Yasaman Ghadar, Scott Parker, Chris Knight, Colleen Bertoni, Thomas Applencourt, Ye Luo, Brian Homerding, JaeHyuk Kwack, Vitali A. Morozov, Adrian C. Pope, Esteban M. Rangel, and David Poole at the 2021 Exascale Computing Project Annual Meeting, April 12-16, 2021.

4. "Overview of the Argonne Aurora Exascale System", Talk presented by Christopher Knight, Yasaman Ghadar, Scott Parker, Kevin Harms, Tim Williams, Katherine Riley, Kalyan Kumaran, Venkat Vishwanath, and James Osborn at the 2021 Exascale Computing Project Annual Meeting, April 12-16, 2021.

5. "Preparing Applications for Aurora", Talk presented by Samuel Williams, Charlene Yang, Jack Deslippe, JaeHyuk Kwack, Christopher Knight, Khaled Ibrahim, and Jonathan Madsen at the 2021 Exascale Computing Project Annual Meeting, April 12-16, 2021.

6. "Portability across Exascale systems", Talk presented at the 3rd Aurora Center of Exellence (COE) Virtual Workshop, Argonne National Laboratory, Oct. 21-22, 2020.

7. "Best Practices for Queueing and Running Jobs on Theta", ALCF Developer Sessions Webinar presented with Adrian Pope and Misha Salim, Argonne National Laboratory, July 29, 2020.

8. "Hybrid Molecular Simulations with LAMMPS", Talk presented at The Platform for Advanced Scientific Computing (PASC) Conference at ETH Zurich, Switzerland, June 12-14, 2019.

9. "Theta Software and Job Submission", Talk presented at ALCF Computational Performance Workshop at Argonne National Laboratory, April 30 - May 2, 2019.

10. "Efficient use of LAMMPS on KNLs", Talk presented at the LCRC "Efficient Use of the KNL Processor" Workshop at Argonne National Laboratory, January 28, 2019.

11. "Preparing Applications for the Argonne Aurora 2021 System", Talk presented with Sudheer, Chunduri, Scott Parker, and Katherine Riley at DOE Exascale Computing Program (ECP) Annual Meeting in Houston, TX, January 14-18, 2019.

12. "Getting Started on ALCF Systems", Talk presented at ALCF Simulation, Data, and Learning Workshop at Argonne National Laboratory, October 2-4, 2018.

13. ”ALCF System Architectures: Software and Job Submission”, Talk presented at ALCF Computational Performance Workshop at Argonne National Laboratory, May 15-17, 2018.

14. ”ALCF System Architectures: Software and Job Submission”, Talk presented at ALCF Computational Performance Workshop at Argonne National Laboratory, May 2-5, 2017.

15. ”Science at ALCF: What has a supercomputer done for me lately?,” Seminar presented at the Undergraduate Student Summer Research Lunch at Benedictine University, June 22, 2016.

16. ”Algorithms for computationally efficient molecular simulations: chemical reactivity, predictive modeling of zeolites, and x-ray damage mechanisms,” LANS Informal Seminar presented at Argonne National Laboratory, October 1, 2014.

17. ”Algorithms for computationally efficient molecular simulations: chemical reactivity, predictive modeling of zeolites, and x-ray damage mechanisms,” Seminar presented at the Argonne Leadership Computing Facility, Argonne National Laboratory, September 3, 2014.

18. ”Computationally efficient reactive models derived from condensed phase ab initio simulations,” Invited talk presented as the Technologies for Extreme Scale Computing seminar in the Center for Computation & Technology at Louisiana State University, July 17, 2014.

19. ”Computationally efficient reactive models derived from condensed phase ab initio simulations”, Seminar presented in the Chemistry Department at the University of Kansas, December 12, 2013.

20. ”Rigorous route to interaction potentials for reactive models derived from condensed phase ab initio simulations”, Talk presented at the 5th Annual Postdoctoral Research Symposium, Argonne National Laboratory, September 20, 2012.

21. ”Rigorous route to interaction potentials for reactive models derived from condensed phase ab initio simulations”, Invited talk presented at the 244th American Chemical Society National Meeting in symposium titled ”Potential energy surface exploration in quantum chemistry” honoring Berny Schlegel, Philadelphia, PA, August 19-23, 2012.

22. ”Extending Parallel Scalability of LAMMPS and Multiscale Reactive Simulations”, Talk presented at XSEDE12, Chicago, IL, July 16-20, 2012.

23. “Defining reactive forcefields from condensed phase ab initio simulations”, Poster presented at the Gordon Research Conference on Batteries, Ventura, CA, March 4-9, 2012.

24. “Defining reactive forcefields from condensed phase ab initio simulations”, Poster presented at the American Conference on Theoretical Chemistry, Telluride, CO, July 17-22, 2011.

25. “Hydrogen bond topology, new interpretations of order/disorder transitions in ice, and the behavior of defects in a disordered ice lattice”, Poster presented at 11th International Conference on the Physics and Chemistry of Ice, Bremerhaven, Germany, July 23-28, 2006.

26. “Hydrogen bond topology, new interpretations of order/disorder transitions in ice, and the behavior of defects in a disordered ice lattice”, Talk presented at 38th Midwest Theoretical Chemistry Conference, Columbus, OH, June 15-17, 2006.

27. “Hydrogen bond topology, new interpretations of order/disorder transitions in ice, and the behavior of defects in a disordered ice lattice”, Talk presented at Midwest Thermodynamics and Statistical Mechanics Conference, Akron, OH, May 25-26, 2006.

28. “Theoretical characterization of the potential energy surfaces of 2-(3-benzylamino-propanoylamino) benzamide”, Poster presented at 225th American Chemical Society National Meeting, New Orleans, LA, March 23-27, 2003.

29. “Microwave synthesis and investigation of medium-sized ring systems containing nitrogen atoms”, Poster presented at 225th American Chemical Society National Meeting, New Orleans, LA, March 23-27, 2003.

Workshops (excluding ALCF training events since joining as staff)

1. Participation in the Nanoporous Materials Genome Center (NMGC) All-Hands meeting hosted by the University of Minnesota, April 4-5, 2022.

2. Participation in the Nanoporous Materials Genome Center (NMGC) Virtual All-Hands meeting hosted by the University of Minnesota, September 13-14, 2021.

3. Participation in the Nanoporous Materials Genome Center (NMGC) All-Hands meeting hosted by the University of Minnesota, October 2-3, 2015.

4. Participation in the 2015 Scientific Discovery through Advanced Computing (SciDAC-3) Principle Investigator Meeting, Bethesda, MD, July 22-24, 2015 and assisted with presenting dual-LCF (ALCF & OLCF) posters.

5. Participation in the Nanoporous Materials Genome Center (NMGC) All-Hands meeting hosted by the University of Minnesota, October 18-19, 2014.

6. Participation as an ALCF Catalyst at the ”Mira Performance Boot Camp” organized by the Argonne Leadership Computing Facility (ALCF), May 20-22, 2014, Argonne National Laboratory.

7. Invitation to participate in the ”7th Bishop’s Lodge Workshop: Materials for Energy Conversion” workshop organized by Plamen Atanassov (The University of New Mexico), November 3-5, 2013, Santa Fe, NM. Talk titled ”Progress towards a fundamental understanding of charge transport mechanisms in fuel cell membranes”.

8. Invitation to participate in the ”ONETEP Master Class 2013” workshop organized by the ONETEP Developers group, August 27-30, 2013, Cambridge, UK.

9. Participation in the ”Mira Performance Boot Camp” organized by the Argonne Leadership Computing Facility (ALCF), May 21-24, 2013, Argonne National Laboratory.

10. Talk titled ”Multiscale Molecular Simulations at the Petascale” at the ”Early Science Program Principle Investigators Meeting” organized by the Argonne Leadership Computing Facility (ALCF), May 15-16, 2013, Argonne National Laboratory.

11. Participation in the ”Mira Community Conference” organized by the Argonne Leadership Computing Facility (ALCF), March 4-8, 2013, Argonne National Laboratory.

12. Invitation to participate in the ”ONETEP Master Class 2012” workshop organized by the ONETEP Developers group, August 28-31, 2012, Cambridge, UK.

13. Invitation to participate in the ”Leadership Computing Platforms, Extreme-scale Applications, and Performance Strategies” workshop organized by the Center for Scalable Application Development Software (CScADS), July 23-26, 2012, Snowbird, UT.

14. Participation in the "Early Science April Workshop - Code for Q" workshop organized by the Argonne Leadership Computing Facility (ALCF), April 30 - May 3, 2012, Argonne National Laboratory.

15. Participation in the "ALCF 2012 Winter Workshop" organized by the Argonne Leadership Computing Facility (ALCF), January 23-26, 2012, Argonne National Laboratory.

16. Talk titled "Multiscale Molecular Simulations at the Petascale" at the "ALCF Early Science Program Kick-Off Workshop" organized by the Argonne Leadership Computing Facility (ALCF), October 18-19, 2010, Argonne National Laboratory.

Funded Projects

1. DOE BES CCS, Lead PI Laura Gagliardi with co-PIs Cong Liu and Christopher Knight, "Exascale Multireference Wave Function Theory Method for Polymer Upcycling Catalysis", FY23-25.

2. DOE BES CCS, Lead PI Ilja J. Siepmann with co-PIs Jason Goodpaster, Sapna Sarupria, Donald Truhlar, Christopher Knight, Alvaro Vazquez-Mayagoitia, Jingyun Ye, David Sholl, Randall Snurr, Laura Gagliardi, Coray Colina, David Cantu, and Alan Aspuru-Guzik, "Predictive Hierarchical Modeling of Chemical Separations and Transformations in Functional Nanoporous Materials: Synergy of Machine Learning, Molecular Simulation, Electronic Structure Theory, and Experiment", FY22.

DOE LCF Projects (excluding Director's Discretionary)

1. Phay Ho, Christopher Knight, and Adam Fouda "Multimodal Imaging with Intense X-ray Pulses", 316,000 node-hours on Theta (ALCF), ALCC 2021-2022.

2. Ahren Jasper, Daniel Moberg, and Chris Knight "Stochastic A Priori Dynamics for Complex Reactive Chemical Environments", 100,000 node-hours on Theta (ALCF), ALCC 2020-2021.

3. J. Ilja Siepmann, Coray Colina, Laura Gagliardi, and Chris Knight "Predictive Modeling of Nanoporous Materials and Multi-phase Systems", 220,000 node-hours on Theta (ALCF), ALCC 2020-2021.

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