Eva **Zurek**

Professor of Chemistry

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Appointments

Professor — *University at Buffalo, SUNY*
Department of Chemistry — *8/2016 – present*

Adjunct Professor — *University at Buffalo, SUNY*
Chemical and Biological Engineering — *9/2019 – present*

Adjunct Professor — *University at Buffalo, SUNY*
Department of Physics — *9/2021 – present*

Associate Professor — *University at Buffalo, SUNY*
Department of Chemistry — *8/2014 – 8/2016*

Assistant Professor — *University at Buffalo, SUNY*
Department of Chemistry — *8/2009 – 8/2014*

Research Interests

- Theoretical and computational materials chemistry
- High pressure science
- Crystal structure prediction
- Superconducting, superhard, 2D, quantum, planetary and catalytic materials
- Solvated electrons and electrides
- Machine learning
- Chemical bonding

Distinctions

2022	**Elected Fellow**, American Physical Society (APS)
2019-2022	**Media interviews**, *Scientific American*, *New York Times*, *Science Friday*, *Quirks & Quarks* and more
2022-2026	**Elected Chair-Line**, American Physical Society Division of Computational Physics (APS-DCOMP)
2019-2022	**Member at Large**, American Physical Society Division of Computational Physics (APS-DCOMP)
2017-2021	**Section Editor**, *Electronic Structure*, Journal of Physics: Condensed Matter
2021-	**Editorial Board Member**, Physical Review Materials
2020-	**Associate Editor**, AIP Advances
2021	**Chancellor's Award for Excellence in Scholarship**, State University of New York (SUNY)
2016	**APT Teaching Award**, University at Buffalo
2014	**Promising Young Scientist Award of CMOA**, Quantum Systems in Chemistry and Physics (QSCP)
2014	**Exceptional Scholar (Young Investigator)**, University at Buffalo, SUNY
2014	**Young Leader Professional Development Award**, The Minerals, Metals & Materials (TMS) Society
2013	**Alfred P. Sloan Research Fellowship**, Sloan Foundation
2002-2006	**PhD Fellowship**, International Max Planck Research School for Advanced Materials
2002	**Masters Studies Scholarship**, University of Calgary
2001-2002	**Alberta Ingenuity Award**, University of Calgary
2001-2002	**Graduate Research Scholarship**, University of Calgary
1999-2000	**Undergraduate NSERC**, University of Calgary
1997-1999	**EGC Family Bursaries in Chemistry**, University of Calgary
1994	**Copp Family Scholarship**, University of Calgary
1994	**Canada Scholarship**, University of Toronto
1994	**Rutherford Scholarship**, Government of Alberta

Professional Preparation

Post Doctoral Research — *Cornell University*
Roald Hoffmann's Group — *1/2008 – 8/2009*

Doctoral & Post Doctoral Research — *Max Planck Institute for Solid State Research, Germany*
Abteilung Andersen — *11/2002 – 12/2007*

Graduate Research & Teaching Assistant — *University of Calgary, Canada*
Department of Chemistry — *5/2000 – 10/2002*

Undergraduate Research — *University of Calgary, Canada*
Department of Chemistry — *9/1999 – 1/2000*

Summer Internship — *Arnhem, The Netherlands*
Akzo Nobel — *6/1999 – 9/1999*

Post-Secondary Education

PhD (Dr. rer. nat.) in Chemistry — *University of Stuttgart, Germany*
Theoretical Chemistry — *11/2002 – 8/2006*

Masters of Science — *University of Calgary, Canada*
Theoretical Chemistry — *9/2000 – 10/2002*

Bachelors of Science — *University of Calgary, Canada*
Chemistry — *9/1994 – 5/2000*

Bachelors of Science — *University of Calgary, Canada*
Physics — *9/1994 – 5/2000*

External Research Funding

Total costs are listed

Current

- $106,219 *Conventional Nanostructured Superconductors through First-Principles Calculations* — 9/1/23 – 8/31/24
  PI: Eva Zurek, co-PI: none
  Intellectual Ventures, Deep Science Fund
- $389,887 (Zurek), *High Energy Density Quantum Matter* — 9/1/23 – 8/21/26
  PI: Gilbert Collins (University of Rochester), UB Senior Personnel: Zurek
  Department of Energy, Fusion Energy Sciences, Quantum Information Sciences
- $104,570 (Zurek), $18M (total) — 10/1/23 – 9/30/26
  Midscale RI-1 (M1:DP): OMEGA EP-Pumped Optical Parametric Amplifier Line (EP OPAL)
  PI: Jonathan Zuegel (Rochester), co-PIs: Zurek, Di Piazza, Dollar, Aprahamian
  NSF, Mid-scale Research Infrastructure-1 program
- $350,337 (Zurek), $10M (total) — 7/1/24 - 6/31/28
  Chicago/DOE Alliance Center (CDAC): A Center of Excellence for Materials at Extremes
  PI: Russell Hemley (University of Illinois at Chicago), Partner: Zurek
  National Nuclear Security Administration, Stewardship Science Academic Alliances Program
- $245,867 (Zurek), $8M (total) — 6/1/20 - 5/31/24
  Chicago/DOE Alliance Center (CDAC): A Center of Excellence for High Pressure Science and Technology
  PI: Russell Hemley (University of Illinois at Chicago), Partner: Zurek
  National Nuclear Security Administration, Stewardship Science Academic Alliances Program

- $500,000 (Zurek), $12.96M (total) *Center for Matter at Atomic Pressures* 8/15/20 – 7/31/25
  PI: Gilbert Collins (University of Rochester), UB Senior Personnel: Zurek
  NSF, Physics Frontier Centers
- $1,184,750 (Zurek), $7.5M (total) *SPICES: SPInodal-hardened high-entropy CEramicS* 5/1/21 – 4/3/26
  PI: Stefano Curtarolo (Duke), co-PIs: Fahrenholtz, Zurek, Brenner, Maria, Wolfe
  Office of Naval Research FY2021 MURI solicitation
- $4020 (Zurek), $1.3M (total) *New Methods for Nitrogen and Oxygen Heterocycle Synthesis* 7/1/20 – 6/30/24
  PI: Sherry Chemler (UB), Co-Investigator: Zurek; NIH
- $485,439 (Zurek), $1.8M (total) 10/1/21 – 9/30/25
  Collaborative Research: DMREF:
  Machine Learning Algorithm Prediction and Synthesis of Next Generation Superhard Functional Materials
  PI: Russell Hemley (University of Illinois at Chicago), co-PIs: Zurek, Kadkhodaei, Trenary
  NSF, DMREF program
- $395,000 *Theoretical Prediction of Hydrogen Rich High-Temperature Superconductors* 8/1/22 – 7/31/25
  PI: Eva Zurek, co-PI: none
  NSF, Division of Materials Research: Condensed Mater Materials Theory program
- $33,155 (Zurek), $900,000 (total) 8/1/22 – 7/31/25
  Partnership for Research and Education on Molecules at High Pressures
  PI: Guang-Lin Zhao (Southern University and A&M College), co-PI: Gilbert Collins (Rochester)
  NSF, Partnership for Research and Education in Physics program

Pending

- $224,000 (Zurek), $600k (total) 6/1/24 – 5/30/27
  Innovative Resources: Development of QuaNSAES, an Integrated Software Platform for Quantum Crystallography Research in Earth Science
  PI: Przemyslaw Dera (University of Hawaii, Manoa), co-PI: Zurek
  NSF, EAR program

Past

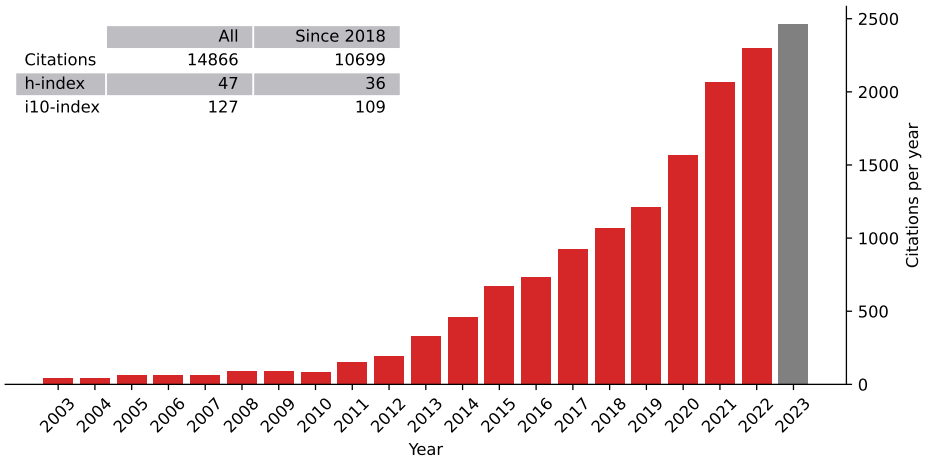
- $100,000 (Zurek), $300,000 (total) 8/15/21 – 8/14/23
  EAGER: SUPER: Collaborative Research:
  Stabilization of Warm and Light Superconductors at Low Pressures by Chemical Doping
  PI: Eva Zurek, co-PIs: Jung-Fu Lin and Jianshi Zhou (UT Austin)
  NSF, Early-concept Grants for Exploratory Research (EAGER) program
- $450,000 (Zurek), $4M (total) *High Energy Density Quantum Matter* 9/1/19 – 8/21/23
  PI: Gilbert Collins (University of Rochester), UB Senior Personnel: Zurek
  Department of Energy, Fusion Energy Sciences, Quantum Information Sciences (1yr NCE)
- $375,000 *Metallization of Hydrogen-Rich Materials: Predicting Novel Superconductors* 1/1/19 – 12/31/22
  PI: Eva Zurek, co-PI: none
  NSF, Division of Materials Research: Condensed Mater Materials Theory program (1yr NCE)
- $20,000 (Zurek), $100,000 (total) *NSF-CREST II Partnership Supplement 2021* 9/1/21 – 8/31/22
  PI: Kimberly Cousins (CSUSB), Subcontract to Zurek; NSF, HRD program
- $106,129 (Zurek) *CDAC: A Center of Excellence for High Pressure Science and Technology* 10/1/18 – 5/1/20
  PI: Steven Gramsch (George Washington University), Partner: Zurek
  National Nuclear Security Administration, Stewardship Science Academic Alliances Program
- $43,500 (Zurek) *CSUSB Center for Materials Science* 1/31/18 – 1/31/20
  PI: Tim Usher (CSUSB), Subcontract to Zurek; NSF, HRD program
- $195,250 (Zurek) *High-throughput prediction of high-pressure materials properties for the AFLOWLIB database* 5/1/16 – 10/31/19
  PI: Stefano Curtarolo (Duke University), co-PIs: Toher, Zurek; ONR
- $345,000 *Tuning Reactivity, Electronic Structure and Properties via Pressure: Predicting Novel Superconductors* (1yr NCE) 6/15/15 – 5/31/19
  PI: Eva Zurek, co-PI: none; NSF, DMR-CMMT
- $999,900 *MRI: Acquisition of High Performance Computing Infrastructure* 10/1/17 – 9/30/18

to Support Computational and Data-Enabled Science and Engineering
PI: Tom Furlani, co-PIs: Autschbach, Bauman, Chandola, Dupuis, Govindaraju, Hachmann, Halfon, Jones, Kofke, Muldoon, Patra, Dutta, Zola, Errington, Pitman, Bian, Hageman, Rajan, Roesch, Ramanathan, Zurek
NSF, Major Research Instrumentation Program

- $63,682 (Zurek) *RUI: Advancing Electrodeposited Dicyano–Ferriprotoporphyrin as an Electrocatalytic Material Capable of Selectively Oxidizing Hydrogen Sulfide Over Interfering Gasotransmitters* 7/1/13 – 6/30/17
  PI: Jason Bennett (Penn State Erie, The Behrend College), Senior Personnel: Zurek
  NSF, Chemical Measurement and Imaging program
- $42,521 (Zurek) *CSUSB Center for Materials Science* 2/1/17 – 1/31/18
  PI: Tim Usher (CSUSB), Subcontract to Zurek; NSF, HRD program
- $40,474 (Zurek) *CSUSB Center for Materials Science* 3/10/15 – 1/31/16
  PI: Tim Usher (CSUSB), Subcontract to Zurek; NSF, HRD program
- $25,000 (Zurek) *Designing Novel Perovskite Solar Cells from First Principles Calculations* 2/1/15 - 6/30/15
  PI: Eva Zurek; Subcontract to CMI, PI: Mark Swihart
  New York State Center of Excellence in Materials Informatics (CMI) Industry Collaboration Projects
- $50,000 *Alfred P. Sloan Research Fellowship* 9/1/13 – 8/31/15
  PI: Eva Zurek, co-PI: none; Sloan Foundation
- $10,000 (Zurek) *Light trapping in ultra-thin films of lead-free hybrid perovskite layers to enhance solar cell efficiency* 1/24/17 – 1/25/18
  PI: Qin Gan, co-PIs: Swihart, Zurek
  University at Buffalo: RENEW Strategic SEED Investment Opportunity
- $15,000 (Zurek) *Collaboration to Develop Key Capability for Materials Innovation* 4/15/14 - 4/14/15
  PI: David Kofke, co-PI: Zurek
  University at Buffalo: Innovative Micro-Programs Accelerating Collaboration in themes
- $56,464 (Zurek) *Boron Carbide at Extreme Conditions* 3/1/17 – 2/29/18
  PI: Russell Hemley (Carnegie Institute Washington), Subcontract to Zurek
  Carnegie/DOE Alliance Center (CDAC), NNSA-SSAP
- $55,449 (Zurek) *Boron Carbide at Extreme Conditions* 3/1/16 – 2/28/17
  PI: Russell Hemley (Carnegie Institute Washington), Subcontract to Zurek
  Carnegie/DOE Alliance Center (CDAC), NNSA-SSAP
- $55,301 (Zurek) *Boron Carbide at Extreme Conditions* 3/1/15 – 2/29/16
  PI: Russell Hemley (Carnegie Institute Washington), Subcontract to Zurek
  Carnegie/DOE Alliance Center (CDAC), NNSA-SSAP
- $55,301 (Zurek) *Boron Carbide at Extreme Conditions* 3/1/14 – 2/28/15
  PI: Russell Hemley (Carnegie Institute Washington), Subcontract to Zurek
  Carnegie/DOE Alliance Center (CDAC), NNSA-SSAP
- $55,256 (Zurek) *Boron Carbide at Extreme Conditions* 3/1/13 – 2/28/14
  PI: Russell Hemley (Carnegie Institute Washington), Subcontract to Zurek
  Carnegie/DOE Alliance Center (CDAC), NNSA-SSAP
- $100,000 *The Role of the Support in (MAO) Methylaluminoxane Activated Olefin Polymerization* 1/1/12 – 8/31/14
  PI: Eva Zurek, co-PI: none
  American Chemical Society Petroleum Research Fund, Doctoral New Investigators
- $379,998 *Metallization of Hydrogen–Rich Materials: Predicting Novel Superconductors* 9/15/10 – 8/31/14
  PI: Eva Zurek, co-PI: none; NSF DMR-CMMT

Publications

Metrics from Google Scholar / Web of Science: over 14,860 / 11,720 citations, h = 47 / 44. Accessed December 28, 2023.



Journal Articles and Book Chapters

[187] Pandey, P.; Wang, X.; Gupta, H.; Smith, P. W.; Lapsheva, E.; Carroll, P. J.; Booth, C. H.; Minasian, S. G.; Autschbach, J.; Zurek, E.; Schelter, E. J., 'Realization of Organocerium-Based Fullerene Molecular Materials Showing Mott Insulator-Type Behavior', **2023**.
submitted

[186] Roberts, J.; Rijal, B.; Divilov, S.; Maria, J. P.; Fahrenholtz, W. G.; Wolfe, D. E.; Brenner, D. W.; Curtarolo, S.; Zurek, E., 'Machine Learned Interatomic Potentials for Ternary Carbides trained on the AFLOW Database', **2023**.
submitted

[185] Geng, N.; Hilleke, K. P.; Belli, F.; Das, P. K.; Zurek, E., 'Superconductivity in CH_4 and BH_4^- Containing Compounds Derived from the High-Pressure Superhydrides', **2023**.
submitted

[184] Liang, X.; Wei, X.; Zurek, E.; Bergara, A.; Li, P.; Gao, G., 'Design of High-Temperature Superconductors at Moderate Pressures by Alloying AlH_3 or GaH_3', *Matter Radiat. Extremes* **2024**, *9*, 018401.
URL `https://doi.org/10.1063/5.0159590`

[183] Divilov, S.; Eckert, H.; Toher, C.; Friedrich, R.; Zettel, A. C.; Brenner, D. W.; Fahrenholtz, W. G.; Wolfe, D. E.; Zurek, E.; Maria, J. P.; Hotz, N.; Campilongo, X.; Curtarolo, S., 'A Priori Procedure to Establish Spinodal Decomposition in Alloys', **2023**.
submitted

[182] Daigle, S. E.; Curtarolo, S.; Fahrenholtz, W. G.; Maria, J. P.; Wolfe, D. E.; Zurek, E.; Brenner, D. W., 'Interfacial Defect Properties of High-Entropy Carbides: Stacking Faults, Shockley Partial Dislocations, and a New Evans-Polanyi-Semenov Relation', **2023**.
submitted

[181] Li, H.; Zhang, Y.; He, J.; Geng, N.; Chariton, S.; Prakapenka, V.; Zurek, E.; Lin, J. F.; Zhou, J., 'Experimental and Theoretical Study of Polytypes to Perovskite Phase Transition in $BaPtO_3$ under High Pressure and High Temperature', **2023**.
submitted

[180] Storm, C. V.; Racioppi, S.; Duff, M. J.; McHardy, J. D.; Zurek, E.; McMahon, M. I., 'Experimental Evidence of Interstitial Electron Density in Transparent Dense Sodium', **2023**.
submitted

[179] Peterson, G. G. C.; Hilleke, K. P.; Lotfi, S.; Zurek, E.; Brgoch, J., 'Twists and Puckers: Tuning Crystal Chemistry in the La(Au_xGe_{1-x})$_2$ Compositional Series', *J. Am. Chem. Soc.* **2023**, *145*, 21612–21622.
URL https://doi.org/10.1021/jacs.3c07936

[178] Divilov, S.; Eckert, H.; Hicks, D.; Oses, C.; Toher, C.; Friedrich, R.; Esters, M.; Mehl, M. J.; Zettel, A. C.; Lederer, Y.; Zurek, E.; Maria, J.-P.; Brenner, D. W.; Campilongo, X.; Filipovic, S.; Fahrenholtz, W. G.; Ryan, C. J.; DeSalle, C. M.; Crealese, R. J.; Wolfe, D. E.; Calzolari, A.; Curtarolo, S., 'Disordered enthalpy-entropy descriptor for high-entropy ceramics discovery', *Nature* **2024**.
URL https://doi.org/10.1038/s41586-023-06786-y

[177] Racioppi, S.; Storm, C. V.; McMahon, M. I.; Zurek, E., 'On the Electride Nature of Na-hP4', *Angew. Chem. Int. Ed.* **2023**, *135*, e202310802.
URL https://doi.org/10.1002/ange.202310802

[176] Wang, B.; Hilleke, K. P.; Hajinazar, S.; Frapper, G.; Zurek, E., 'Structurally Constrained Evolutionary Algorithm for the Discovery and Design of Metastable Phases', *J. Chem. Theory Comput.* **2023**, *19*, 7960–7971.
URL https://doi.org/10.1021/acs.jctc.3c00594

[175] Hilleke, K. P.; Wang, X.; Luo, D.; Geng, N.; Wang, B.; Belli, F.; Zurek, E., 'Structure, Stability and Superconductivity of N-doped Lutetium Hydrides at kbar Pressures', *Phys. Rev. B* **2023**, *108*, 014511 (1–12).
URL http://doi.org/10.1103/PhysRevB.108.014511

[174] Racioppi, S.; Miao, M.; Zurek, E., 'Intercalating Helium into A-site Vacant Perovskites', *Chem. Mater.* **2023**, *35*, 4297–4310.
URL https://doi.org/10.1021/acs.chemmater.3c00353

[173] Wei, X.; Hao, X.; Bergara, A.; Zurek, E.; Liang, X.; Wang, L.; Song, X.; Li, P.; Wang, L.; Gao, G.; Tian, Y., 'Designing Ternary Superconducting Hydrides with A15-type Structure at Moderate Pressures', *Mater. Today Phys.* **2023**, *34*, 101086.
URL https://doi.org/10.1016/j.mtphys.2023.101086

[172] Hanson, M. D.; Miller, D. P.; Kondeti, C.; Brown, A.; Zurek, E.; Simpson, S., 'A Computational Experiment Introducing Undergraduates to Geometry Optimizations, Vibrational Frequencies, and Potential Energy Surfaces', *J. Chem. Educ.* **2023**, *100*, 921–927.
URL https://doi.org/10.1021/acs.jchemed.2c01129

[171] Fang, M.; Kumar, G. S.; Racioppi, S.; Zhang, H.; Zurek, E.; Lin, Q., 'Hydrazonyl Sultones as Stable Tautomers of Highly Reactive Nitrile Imines for Fast Bioorthogonal Ligation Reaction', *J. Am. Chem. Soc.* **2023**, *145*, 9959–9964.
URL https://doi.org/10.1021/jacs.2c12325

[170] Geng, N.; Hilleke, K. P.; Zhu, L.; Wang, X.; Strobel, T. A.; Zurek, E., 'Conventional High-Temperature Superconductivity in Metallic, Covalently Bonded, Binary-Guest C-B clathrates', *J. Am. Chem. Soc.* **2023**, *145*, 1696–1706.
URL https://doi.org/10.1021/jacs.2c10089

[169] Wolfe, D. E.; DeSalle, C. M.; Ryan, C. J.; Slapikas, R. E.; Sweny, R. T.; Crealese, R. J.; Kolonin, P. A.; Stepanoff, S. P.; Haque, A.; Divilov, S.; Eckert, H.; Oses, C.; Esters, M.; Brenner, D. W.; Fahrenholtz, W. G.; Maria, J.-P.; Toher, C.; Zurek, E.; Curtarolo, S., 'Influence of Processing on the Microstructural Evolution and Multiscale Hardness in Titanium Carbonitrides (TiCN) Produced via Field Assisted Sintering Technology', *Materiala* **2023**, *27*, 101682.
URL https://doi.org/10.1016/j.mtla.2023.101682

[168] Hilleke, K. P.; Zurek, E., '3.13 - Crystal chemistry at high pressure', in Reedijk, J.; Poeppelmeier, K. R. (editors), 'Comprehensive Inorganic Chemistry III (Third Edition)', Elsevier, Oxford, third edition edition, **2023**, 421–445.
URL https://www.sciencedirect.com/science/article/pii/B9780128231449001709

[167] Antle, J. P.; Kimura, M. W.; Racioppi, S.; Damon, C.; Lang, M.; Gatley-Montross, C.; Sanchez B, L. S.; Miller, D. P.; Zurek, E.; Brown, A. M.; Gast, K.; Simpson, S. M., 'Applying Density Functional Theory to Common Organic

Mechanisms: A Computational Exercise', *J. Chem. Educ.* **2023**, *100*, 355–360.
URL https://doi.org/10.1021/acs.jchemed.2c00935

[166] Hilleke, K. P.; Franco, R.; Pertierra, P.; Salvado, M. A.; Zurek, E.; Recio, J. M., 'Preference for a Pressure-Induced Orthorhombic Structure after 1T-$HfSe_2$', *Mater. Today Phys.* **2023**, *36*, 101152.
URL https://doi.org/10.1016/j.mtphys.2023.101152

[165] Oses, C.; Esters, M.; Hicks, D.; Divilov, S.; Eckert, H.; Friedrich, R.; Mehl, M. J.; Smolyanyuk, A.; Campilongo, X.; van de Walle, A.; Schroers, J.; Kusne, A. G.; Takeuchi, I.; Zurek, E.; Nardelli, M. B.; Fornari, M.; Lederer, Y.; Levy, O.; Toher, C.; Curtarolo, S., 'aflow++: A C++ Framework for Autonomous Materials Design', *Comput. Mater. Sci.* **2023**, *217*, 111889.
URL https://doi.org/10.1016/j.commatsci.2022.111889

[164] Sobiech, T. A.; Zhong, Y.; Miller, D. P.; McGrath, J. K.; Scalzo, C. T.; Redington, M. C.; Zurek, E.; Gong, B., 'Ultra-Tight Host-Guest Binding with Exceptionally Strong Positive Cooperativity', *Angew. Chem. Int. Ed.* **2022**, *61*, e202213467.
URL https://doi.org/10.1002/anie.202213467

[163] Hilleke, K.; Zurek, E., 'Rational Design of Superconducting Metal Hydrides via Chemical Pressure Tuning', *Angew. Chem. Int. Ed.* **2022**, *61*, e202207589.
URL https://doi.org/10.1002/anie.202207589

[162] Wang, B.; Hilleke, K. P.; Wang, X.; Polsin, D. N.; Zurek, E., 'Topological Electride Phase of Sodium at High Pressures and Temperatures', *Phys. Rev. B* **2023**, *107*, 184101.
URL https://doi.org/10.1103/PhysRevB.107.184101

[161] Roberts, J.; Zurek, E., 'Computational Materials Discovery', *J. Chem. Phys.* **2022**, *156*, 210401.
URL https://doi.org/10.1063/5.0096008

[160] Wang, X.; Proserpio, D. M.; Oses, C.; Toher, C.; Curtarolo, S.; Zurek, E., 'The Microscopic Diamond Anvil Cell: Stabilization of Superhard, Superconducting Carbon Allotropes at Ambient Pressure', *Angew. Chem. Int. Ed.* **2022**, *61*, e202205129.
URL https://doi.org/10.1002/anie.202205129

[159] Yang, H. J.; Redington, M.; Miller, D. P.; Zurek, E.; Kim, M.; Yoo, C.-S.; Lim, S. Y.; Cheong, H.; Chae, S.-A.; Ahn, D.; Hur, N. H., 'New Monoclinic Ruthenium Dioxide with Highly Selective Hydrogenation Activity', *Catal. Sci. Technol.* **2022**, *12*, 6556.
URL https://doi.org/10.1039/d2cy00815g

[158] Cao, R.; Rossdeutcher, R. B.; Zhong, Y.; Shen, Y.; Miller, D. P.; Sobiech, T. A.; Wu, X.; Sanchez Buitrago, L.; Ramcharan, K.; Gutay, M. I.; Frankenthal Figueira, M.; Luthra, P.; Zurek, E.; Szyperski, T.; Button, B.; Shao, Z.; Gong, B., 'Aromatic Pentaamide Macrocycles Bind Anions with High Affinity for Transport Across Biomembranes', *Nat. Chem* **2023**, *15*, 1559–1568.
URL https://doi.org/10.1038/s41557-023-01315-w

[157] Schunke, C.; Miller, D. P.; Zurek, E.; Morgenstern, K., 'Halogen and Structure Sensitivity of Halobenzene Adsorption on Copper Surfaces', *Phys. Chem. Chem. Phys.* **2022**, *24*, 4485–4492.
URL https://doi.org/10.1039/d1cp05660c

[156] Geng, N.; Bi, T.; Zurek, E., 'Structural Diversity and Superconductivity in S-P-H Ternary Hydrides Under Pressure', *J. Phys. Chem. C* **2022**, *126*, 7208–7220.
URL https://doi.org/10.1021/acs.jpcc.1c10976

[155] Hilleke, K. P.; Bi, T.; Zurek, E., 'Materials Under High Pressure: A Chemical Perspective', *J. Appl. Phys.* **2022**, *128*, 441.
URL https://doi.org/10.1007/s00339-022-05576-z

[154] Zhang, S.; Morales, M. A.; Jeanloz, R.; Millot, M.; Hu, S. X.; Zurek, E., 'Nature of the Bonded-to-Atomic Transition in Liquid Silica to TPa Pressures', *J. Appl. Phys.* **2022**, *131*, 071101.
URL https://doi.org/10.1063/5.0081293

[153] Breeman, B.; Tiglias, A. T.; Mancuso, J.; Zurek, E.; Miller, D. P.; Velarde, L., 'Insight into the Adsorption Structure of TIPS-Pentacene on Noble Metal Surfaces', *J. Phys. Chem. C* **2022**, *126*, 2689–2698.
URL https://doi.org/10.1021/acs.jpcc.1c10283

[152] Hilleke, K. P.; Zurek, E., 'Tuning Chemical Precompression: Theoretical Design and Crystal Chemistry of Novel Hydrides in the Quest for Warm and Light Superconductivity at Ambient Pressures', *J. Appl. Phys.* **2022**, *131*, 070901.
URL https://doi.org/10.1063/5.0077748

[151] Kumar, G. S.; Racioppi, S.; Zurek, E.; Lin, Q., 'Superfast Tetrazole-BCN Cycloaddition Reaction for Bioorthogonal Protein Labelling in Live Cells', *J. Am. Chem. Soc.* **2022**, *144*, 57–62.
URL https://doi.org/10.1021/jacs.1c10354

[150] Wang, X.; Bi, T.; Hilleke, K. P.; Lamichhane, A.; Hemley, R. J.; Zurek, E., 'Dilute Carbon in H_3S Under Pressure', *npj Comput. Mater.* **2022**, *8*, 87 (1–9).
URL https://doi.org/10.1038/s41524-022-00769-9

[149] Sobiech, T. A.; Zhong, Y.; Sanchez B, L. S.; Kauffmann, B.; McGrath, J. K.; Scalzo, C.; Miller, D. P.; Huc, I.; Zurek, E.; Ferrand, Y.; Gong, B., 'Stable Pseudo[3]rotaxanes with Strong Positive Binding Cooperativity Based on Shape-Persistent Aromatic Oligoamide Macrocycles', *Chem. Commun.* **2021**, *57*, 11645–11648.
URL https://doi.org/10.1039/d1cc05193h

[148] Bertram, C.; Miller, D. P.; Schunke, C.; Kemeny, I.; Kimura, M. W.; Bovensiepen, U.; Zurek, E.; Morgenstern, K., 'Interplay of Halogen and Weak Hydrogen Bonds in the Formation of Magic Nanoclusters on Surfaces', *J. Phys. Chem. C* **2022**, *126*, 588–596.
URL https://doi.org/10.1021/acs.jpcc.1c08045

[147] Berhane, I.; Burde, A. S.; Kennedy-Ellis, J. J.; Zurek, E.; Chemler, S. R., 'Copper-Catalyzed Enantioselective Alkene Carboetherification for the Synthesis of Saturated Six-Membered Cyclic Ethers', *Chem. Commun.* **2021**, *57*, 10099–10102.
URL https://doi.org/10.1039/d1cc03515k

[146] Yu, X.; Zhou, T.; Zhao, Y.; Lu, F.; Zhang, X.; Liu, G.; Gou, H.; Zurek, E.; Luo, X., 'Surface Magnetism in Pristine α Rhombohedral Boron and Intersurface Exchange Coupling Mechanism of Boron Icosahedra', *J. Phys. Chem. Lett.* **2021**, *12*, 6812–6817.
URL https://doi.org/10.1021/acs.jpclett.1c01860

[145] Yang, Q.; Lin, J.; Li, F.; Zhang, J.; Zurek, E.; Yang, G., 'Pressure-Induced Yttrium Oxides with Unconventional Stoichiometries and Novel Properties', *Phys. Rev. Materials* **2021**, *5*, 044802 (1–7).
URL https://doi.org/10.1103/PhysRevMaterials.5.044802

[144] Sun, X.; Zhong, Y.; Li, Y.-H.; Miller, D. P.; Buttan, S.; Wu, X.-X.; Zhang, Y.; Tang, Q.; Tan, H.-W.; Zhu, J.; Liu, R.; Zurek, E.; Lu, Z.-L.; Gong, B., 'Reliable Folding of Hybrid Tetrapeptides into Short beta-Hairpins', *Chin. Chem. Lett.* **2021**, *33*, 257–261.
URL https://doi.org/10.1016/j.cclet.2021.06.019

[143] Hilleke, K. P.; Ogitsu, T.; Zhang, S.; Zurek, E., 'Structural Motifs and Bonding in Two Families of Boron Structures Predicted at Megabar Pressures', *Phys. Rev. Materials* **2021**, *5*, 053605.
URL https://doi.org/10.1103/PhysRevMaterials.5.053605

[142] Kurzydlowski, D.; Derzsi, M.; Zurek, E.; Grochala, W., 'Fluorides of Silver Under Large Compression', *Chem. Eur. J.* **2021**, *27*, 5536–5545.
URL https://doi.org/10.1002/chem.202100028

[141] Bi, T.; Shamp, A.; Terpstra, T.; Hemley, R. J.; Zurek, E., 'The Li-F-H Ternary System at High Pressures', *J. Chem. Phys.* **2021**, *154*, 124709 (1–11).
URL https://doi.org/10.1063/5.0041490

[140] Swanson, W. B.; Tabaczynski, D.; Lis, D.; Zurek, E.; Kozik, M., 'Direct Experimental ^{31}P 2D DOSY NMR Evidence for Oligomerization of Transition-Metal Substituted Polyoxotungstates in Nonpolar Solvents', *Polyhe-*

dron **2021**, *204*, 115174.
URL https://doi.org/10.1016/j.poly.2021.115174

[139] Lilia, B.; Hennig, R.; Hirschfeld, P.; Profeta, G.; Sanna, A.; Zurek, E.; Pickett, W. E.; Amsler, M.; Dias, R.; Eremets, M. I.; Heil, C.; Hemley, R. J.; Liu, H.; Ma, Y.; Pierleoni, C.; Kolmogorov, A. N.; Rybin, N.; Novoselov, D.; Anisimov, V.; Oganov, A. R.; Pickard, C. J.; Bi, T.; Arita, R.; Errea, I.; Pellegrini, C.; Requist, R.; Gross, E. K. U.; Margine, E. R.; Xie, S. R.; Quan, Y.; Hire, A.; Fanfarillo, L.; Stewart, G. R.; Hamlin, J. J.; Stanev, V.; Gonnelli, R. S.; Piatti, E.; Romanin, D.; Daghero, D.; Valenti, R., 'The 2021 Room-Temperature Superconductivity Roadmap', *J. Phys. Condens. Mat.* **2022**, *34*, 183002.
URL https://doi.org/10.1088/1361-648x/ac2864

[138] Snider, E.; Dasenbrock-Gammon, N.; McBride, R.; Wang, X.; Meyers, N.; Lawler, K. V.; Zurek, E.; Salamat, A.; Dias, R. P., 'Synthesis of Yttrium Superhydride Superconductor with a Transition Temperature up to 262 K by Catalytic Hydrogenation at High Pressures', *Phys. Rev. Lett.* **2021**, *126*, 117003 (1–6).
URL https://doi.org/10.1103/PhysRevLett.126.117003

[137] Falls, Z.; Avery, P.; Wang, X.; Hilleke, K. P.; Zurek, E., 'The XtalOpt Evolutionary Algorithm for Crystal Structure Prediction', *J. Phys. Chem. C* **2021**, *125*, 1601–1620.
URL https://doi.org/10.1021/acs.jpcc.0c09531

[136] Riedel, R.; Seel, A. G.; Malko, D.; Miller, D. P.; Sperling, B. T.; Choi, H.; Headen, T. F.; Zurek, E.; Porch, A.; Kucernak, A.; Pyper, N. C.; Edwards, P. P.; Barrett, A. G. M., 'Superalkali-Alkalide Interactions and Ion Pairing in Low-Polarity Solvents', *J. Am. Chem. Soc.* **2021**, *143*, 3934–3943.
URL https://doi.org/10.1021/jacs.1c00115

[135] Yan, Y.; Bi, T.; Geng, N.; Wang, X.; Zurek, E., 'A Metastable $CaSH_3$ Phase Composed of HS Honeycomb Sheets that is Superconducting Under Pressure', *J. Phys. Chem. Lett.* **2020**, *11*, 9629–9636.
URL https://doi.org/10.1021/acs.jpclett.0c02299

[134] Cai, W.; Lin, W.; Yan, Y.; Hilleke, K. P.; Coles, J.; Bao, J.-K.; Xu, J.; Zhang, D.; Chung, D. Y.; Kanatzidis, M. G.; Zurek, E.; Deemyad, S., 'Pressure-Induced Superconductivity in the Wide Band Gap Semiconductor $Cu_2Br_2Se_6$ with a Robust Framework', *Chem. Mater.* **2020**, *32*, 6237–6246.
URL https://doi.org/10.1021/acs.chemmater.0c02151

[133] Cui, X.; Hilleke, K. P.; Wang, X.; Lu, M.; Zhang, M.; Zurek, E.; Li, W.; Zhang, D.; Yan, Y.; Bi, T., 'RbB_3Si_3: An Alkali Metal Borosilicide that is Metastable and Superconducting at 1 atm', *J. Phys. Chem. C* **2020**, *124*, 14826–14831.
URL https://doi.org/10.1021/acs.jpcc.0c04617

[132] Du, Y.; Li, W.; Zurek, E.; Gao, L.; Cui, X.; Zhang, M.; Liu, H.; Tian, Y.; Zhang, S.; Zhang, D., 'Predicted CsSi Compound: A Promising Material for Photovoltaic Applications', *Phys. Chem. Chem. Phys.* **2020**, *22*, 11578–11582.
URL https://doi.org/10.1039/D0CP01440K

[131] Zhong, Y.; Tang, Q.; Miller, D. P.; Zurek, E.; Liu, R.; Lu, Z.-L.; Gong, B., 'Major Factors for the Persistent Folding of Hybrid α, β, γ-Hybrid Peptides into Hairpins', *Front. Chem.* **2020**, *8*, 530083.
URL https://doi.org/10.3389/fchem.2020.530083

[130] Cui, W.; Bi, T.; Shi, J.; Li, Y.; Liu, H.; Zurek, E.; Hemley, R. J., 'Route to High-T_c Superconductivity via CH_4-Intercalated H_3S Hydride Perovskites', *Phys. Rev. B* **2020**, *101*, 134504 (1–5).
URL https://doi.org/10.1103/PhysRevB.101.134504

[129] Bi, T.; Zurek, E., 'Electronic Structure and Superconductivity of Compressed Metal Tetrahydrides', *Chem. Eur. J.* **2021**, *27*, 14848–14870.
URL https://doi.org/10.1002/chem.202102679

[128] Tang, Q.; Zhong, Y.; Miller, D. P.; Liu, R.; Zurek, E.; Lu, Z.-L.; Gong, B., 'Reverse Turn Foldamers: An Expanded β-Turn Motif Reinforced by Double Hydrogen Bonds', *Org. Lett.* **2020**, *22*, 1003–1007.
URL https://dx.doi.org/10.1021/acs.orglett.9b04547

[127] Miao, M.; Sun, Y.; Zurek, E.; Lin, H., 'Chemistry Under High Pressure', *Nat. Rev. Chem.* **2020**, *4*, 508–527.
URL https://doi.org/10.1038/s41570-020-0213-0

[126] Kou, C.; Tian, Y.; Zhang, M.; Zurek, E.; Qu, X.; Wang, X.; Yin, K.; Yan, Y.; Gao, L.; Lu, M.; Yang, W., 'M-graphene: A Metastable Two-Dimensional Carbon Allotrope', *2D Mater.* **2020**, *7*, 025047 (1–7).
URL https://doi.org/10.1088/2053-1583/ab7977

[125] Hu, Y.; Adhikari, D.; Tan, A.; Dong, X.; Zhu, T.; Wang, X.; Huang, Y.; Mitchell, T.; Yao, Z.; Dasenbrock-Gammon, N.; Snider, E.; Dias, R. P.; Huang, C.; Kim, R.; Neuhart, I.; Ali, A. H.; Zhang, J.; Bechtel, H. A.; Martin, M. C.; Corder, S. N. G.; Hu, F.; Li, Z.; Armstrong, J. N.; Wang, J.; Liu, M.; Benedict, J.; Zurek, E.; Sambandamurthy, G.; Grossmann, J. C.; Zhang, P.; Ren, S., 'Laser-Induced Cooperative Transition in Molecular Electronic Crystal', *Adv. Mater.* **2021**, *33*, 2103000.
URL https://doi.org/10.1002/adma.202103000

[124] Wang, Q.; Zhong, Y.; Miller, D. P.; Lu, X.; Tang, Q.; Lu, Z.-L.; Zurek, E.; Liu, R.; Gong, B., 'Self-Assembly and Molecular Recognition in Water: Tubular Stacking and Guest-Templated Discrete Assembly of Water-Soluble, Shape-Persistent Macrocycles', *J. Am. Chem. Soc.* **2020**, *142*, 2915–2924.
URL https://dx.doi.org/10.1021/jacs.9b11536

[123] Zhao, L.; Liu, W.; Yi, W.; Hu, T.; Khodagholian, D.; Gu, F.; Lin, H.; Zurek, E.; Zheng, Y.; Miao, M., 'Nano-Makisu: Highly Anisotropic Two-Dimensional Carbon Allotropes Made by Weaving Together Nanotubes', *Nanoscale* **2020**, *12*, 347–355.
URL https://doi.org/10.1039/c9nr08069d

[122] Selvakumar, J.; Simpson, S. M.; Zurek, E.; Arumugam, K., 'An Electrochemically Controlled Release of NHCs Using Iron Bis(dithiolene) N-heterocyclic Carbene Complexes', *Inorg. Chem. Front.* **2021**, *8*, 59–71.
URL https://doi.org/10.1039/d0qi00638f

[121] Geng, N.; Bi, T.; Zarifi, N.; Yan, Y.; Zurek, E., 'A First-Principles Exploration of Na_xS_y Binary Phases at 1 atm and Under Pressure', *Crystals* **2019**, *9*, 441 (1–17).
URL https://doi.org/10.3390/cryst9090441

[120] Sperling, J. M.; Warzecha, E. J.; Celis-Barros, C.; Sergentu, D.-C.; Wang, X.; Klamm, B. E.; Windorff, C. J.; Gaiser, A. N.; White, F. D.; Beery, D. A.; Chemey, A. T.; Whitefoot, M. A.; Long, B. N.; Hanson, K.; Kögerler, P.; Speldrich, M.; Zurek, E.; Autschbach, J.; Albrecht-Schönzart, T. E., 'Compression of Curium Pyrrolidine-Dithiocarbamate Enhances Covalency', *Nature* **2020**, *583*, 396–399.
URL https://doi.org/10.1038/s41586-020-2479-2

[119] Miller, D. P.; Phillips, A.; Ludowieg, H.; Swihart, S.; Autschbach, J.; Zurek, E., 'The Computational Design of Two-Dimensional Materials', *J. Chem. Educ.* **2019**, *96*, 2308–2314.
URL https://doi.org/10.1021/acs.jchemed.9b00485

[118] Avery, P.; Wang, X.; Oses, C.; Gossett, E.; Proserpio, D. M.; Toher, C.; Curtarolo, S.; Zurek, E., 'Predicting Superhard Materials via a Machine Learning Informed Evolutionary Structure Search', *npj Comput. Mater.* **2019**, *5*, 89 (1–11).
URL https://doi.org/10.1038/s41524-019-0226-8

[117] Zhang, Y.; Zhong, Y.; Connor, A. L.; Miller, D. P.; Cao, R.; Shen, J.; Song, B.; Baker, E. S.; Tang, Q.; Pulavarti, S. V. S. R. K.; Liu, R.; Wang, Q.; Lu, Z.-L.; Szyperski, T.; Zeng, H.; Li, X.; Smith, R. D.; Zurek, E.; Zhu, J.; Gong, B., 'Folding and Assembly of Short α, β, γ-hybrid Peptides: Minor Variations in Sequence and Drastic Differences in Higher-Level Structures', *J. Am. Chem. Soc.* **2019**, *14239-14248*, 141.
URL https://doi.org/10.1021/jacs.9b06094

[116] Zurek, E.; Bi, T., 'High-Temperature Superconductivity in Alkaline and Rare Earth Polyhydrides at High Pressure: A Theoretical Perspective', *J. Chem. Phys.* **2019**, *150*, 050901 (1–13).
URL https://doi.org/10.1063/1.5079225

[115] Zurek, E., 'Pushing Towards Room-Temperature Superconductivity', *Physics* **2019**, *12*, 1.
URL https://doi.org/10.1103/physics.12.1

[114] Li, W.; Lu, M.; Zurek, E.; Xu, X.; Chen, L.; Zhang, M.; Gao, L.; Zhong, X.; Li, J.; Zhou, X.; Liu, W., 'Crystal Structures of Silicon-Rich Lithium Silicides at High Pressure', *Phys. Lett. A* **2019**, *383*, 1047–1051.
URL https://doi.org/10.1016/j.physleta.2018.12.022

[113] Avery, P.; Toher, C.; Curtarolo, S.; Zurek, E., 'XtalOpt version r12: An Open-Source Evolutionary Algorithm for Crystal Structure Prediction', *Comput. Phys. Commun.* **2019**, *237*, 274–275.
URL https://doi.org/10.1016/j.cpc.2018.11.016

[112] Liu, W.; Zhao, L.; Zurek, E.; Xia, J.; Zheng, Y.-H.; Lin, H.-Q.; Liu, J.-Y.; Miao, M.-S., 'Building Egg-Tray-Shaped Graphenes that have Superior Mechanical Strength and Band Gap', *npj Comput. Mater.* **2019**, *5*, 71 (1–8).
URL https://doi.org/10.1038/s41524-019-0211-2

[111] Zarifi, N.; Bi, T.; Liu, H.; Zurek, E., 'Crystal Structures and Properties of Iron Hydrides at High Pressure', *J. Phys. Chem. C* **2018**, *122*, 24262–24269.
URL https://doi.org/10.1021/acs.jpcc.8b06934

[110] Borges-Munoz, A. C.; Miller, D. P.; Zurek, E.; Colon, L., 'Silanization of Superficially Porous Silica Particles with p-Aminophenyltrimethoxysilane', *Microchem. J.* **2019**, *147*, 263–268.
URL https://doi.org/10.1016/j.microc.2019.02.013

[109] Fu, Z. H.; Bi, T. G.; Zhang, S. H.; Chen, S.; Zurek, E.; Legut, D.; German, T. C.; Lookman, T.; Zhang, R. F., 'Anchoring Effect of Distorted Octahedra on the Stability and Strength of Platinum Metal Pernitrides', *Phys. Rev. Mater.* **2019**, *3*, 013603 (1–8).
URL https://doi.org/10.1103/physrevmaterials.3.013603

[108] Bi, T.; Zarifi, N.; Terpstra, T.; Zurek, E., 'The Search for Superconductivity in High Pressure Hydrides', in Reedijk, J. (editor), 'Reference Module in Chemistry, Molecular Sciences and Chemical Engineering', Elsevier, Waltham, MA, **2019**, 1–36.
URL https://doi.org/10.1016/b978-0-12-409547-2.11435-0

[107] Gaffney, J. A.; Hu, S. X.; Arnault, P.; Becker, A.; Benedict, L. X.; Boehly, T. R.; Celliers, P. M.; Ceperley, D. M.; Certik, O.; Clerouin, J.; Collins, G. W.; Collins, L. A.; Danel, J. F.; Desbiens, N.; Dharma-wardana, M. W. C.; Ding, Y. H.; Fernandez-Panella, A.; Gregor, M. C.; Grabowski, P. E.; Hamel, S.; Hansen, S. B.; Harbour, L.; He, X. T.; Johnson, D. D.; Kang, W.; Karasiev, V. V.; Kazandjian, L.; Knudson, M. D.; Ogitsu, T.; Pierleoni, C.; Piron, R.; Redmer, R.; Robert, G.; Saumon, D.; Shamp, A.; Sjostrom, T.; Smirnov, A. V.; Starrett, C. E.; Sterne, P. A.; Wardlow, A.; Whitley, H. D.; Wilson, B.; Zhang, P.; Zurek, E., 'A Review of Equation-of-State Models for Inertial Confinement Fusion Materials', *High Energ. Dens. Phys.* **2018**, *28*, 7–24.
URL https://doi.org/10.1016/j.hedp.2018.08.001

[106] Mishra, A. K.; Muramatsu, T.; Liu, H.; Geballe, Z. M.; Somayazulu, M.; Ahart, M.; Baldini, M.; Meng, Y.; Zurek, E.; Hemley, R. J., 'New Calcium Hydrides with Mixed Atomic and Molecular Hydrogen', *J. Phys. Chem. C* **2018**, *122*, 19370–19378.
URL https://doi.org/10.1021/acs.jpcc.8b05030

[105] Bennett, J. A.; Miller, D. P.; Simpson, S. M.; Rodrigues, M.; Zurek, E., 'Electrochemical Atomic Force Microscopy and First-Principles Calculations of Ferriprotoporphyrin Adsorption and Polymerization', *Langmuir* **2018**, *34*, 11335–11346.
URL https://doi.org/10.1021/acs.langmuir.8b02059

[104] Toher, C.; Oses, C.; Hicks, D.; Gossett, E.; Rose, F.; Nath, P.; Usanmaz, D.; Ford, D. C.; Perim, E.; Calderon, C. E.; Plata, J. J.; Lederer, Y.; Jahnatek, M.; Setyawan, W.; Wang, S.; Xue, J.; Rasch, K.; Chepulskii, R. V.; Taylor, R. H.; Gomez, G.; Shi, H.; Supka, A. R.; Al Orabi, R. A. R.; Gopal, P.; Cerasoli, F. T.; Liyanage, L.; Wang, H.; Siloi, I.; Agapito, L. A.; Nyshadham, C.; Hart, G. L. W.; Carrete, J.; Legrain, F.; Mingo, N.; Zurek, E.; Isayev, O.; Tropsha, A.; Sanvito, S.; Hanson, R. M.; Takeuchi, I.; Mehl, M. J.; Kolmogorov, A. N.; Yang, K.; D'Amico, P.; Calzolari, A.; Costa, M.; De Gennaro, R.; Nardelli, M. B.; Fornari, M.; Levy, O.; Curtarolo, S., 'The AFLOW Fleet for Materials Discovery', in Andreoni, W.; Yip, S. (editors), 'Handbook of Materials Modeling. Volume 1 Methods: Theory and Modeling', Vol. 1, Springer, Cham, Switzerland, **2018**, 1–28.
URL https://doi.org/10.1007/978-3-319-42913-7_63-1

[103] Gossett, E.; Toher, C.; Oses, C.; Isayev, O.; Legrain, F.; Rose, F.; Zurek, E.; Carrete, J.; Mingo, N.; Tropsha, A.; Curtarolo, S., 'AFLOW-ML: A RESTful API for Machine-Learning Predictions of Materials Properties', *Comput. Mater. Sci.* **2018**, *152*, 134–145.
URL https://doi.org/10.1016/j.commatsci.2018.03.075

[102] Zarifi, N.; Liu, H.; Tse, J. S.; Zurek, E., 'Crystal Structures and Electronic Properties of Xe-Cl Compounds at High Pressure', *J. Phys. Chem. C* **2018**, *122*, 2941–2950.
URL https://doi.org/10.1021/acs.jpcc.7b10810

[101] Shelton, H.; Bi, T.; Zurek, E.; Smith, J.; Dera, P., 'The Ideal Crystal Structure of Cristobalite X-I: A Bridge in SiO_2 Densification', *J. Phys. Chem. C* **2018**, *122*, 17437–17446.
URL https://doi.org/10.1021/acs.jpcc.8b04282

[100] Avery, P.; Falls, Z.; Zurek, E., 'XtalOpt Version r11: An Open-Source Evolutionary Algorithm for Crystal Structure Prediction', *Comput. Phys. Commun.* **2018**, *222*, 418–419.
URL https://doi.org/10.1016/j.cpc.2017.09.011

[99] Ye, X.; Zarifi, N.; Zurek, E.; Hoffmann, R.; Ashcroft, N. W., 'High Hydrides of Scandium Under Pressure: Potential Superconductors', *J. Phys. Chem. C* **2018**, *122*, 6298–6309.
URL https://doi.org/10.1021/acs.jpcc.7b12124

[98] Liu, Z.; Botana, J.; Hermann, A.; Valdez, S.; Zurek, E.; Yan, D.; Lin, H.-Q.; Miao, M.-S., 'Reactivity of He with Ionic Compounds Under High Pressure', *Nat. Commun.* **2018**, *9*, 951.
URL https://doi.org/10.1038/s41467-018-03284-y

[97] Avery, P.; Ludowieg, H.; Autschbach, J.; Zurek, E., 'Extended Hückel Calculations on Solids using the Avogadro Molecular Editor and Visualizer', *J. Chem. Educ.* **2018**, *95*, 331–337.
URL https://doi.org/10.1021/acs.jchemed.7b00698

[96] Teeter, J. D.; Costa, P. S.; Pour, M. M.; Miller, D. P.; Zurek, E.; Enders, E.; Sinitskii, A., 'Epitaxial Growth of Aligned Atomically Precise Chevron Graphene Nanoribbons on Cu(111)', *Chem. Commun.* **2017**, *53*, 8463–8466.
URL https://doi.org/10.1039/c6cc08006e

[95] Zhang, R.; Cai, W.; Bi, T.; Zarifi, N.; Terpstra, T.; Zhang, C.; Valy Verdeny, Z.; Zurek, E.; Deemyad, S., 'Effects of Non-Hydrostatic Stress on Structural and Optoelectronic Properties of Methylammonium Lead Bromide Perovskite', *J. Phys. Chem. Lett.* **2017**, *8*, 3457–3465.
URL https://doi.org/10.1021/acs.jpclett.7b01367

[94] Zhang, X.; Costa, P. S.; Hooper, J.; Miller, D. P.; N'Diaye, A. T.; Beniwal, S.; Jiang, X.; Yin, Y.; Rosa, P.; Routaboul, L.; Gonidec, M.; Poggini, L.; Braunstein, P.; Doudin, B.; Xu, X.; Enders, A.; Zurek, E.; Dowben, P. A., 'Locking and Unlocking the Molecular Spin Cross-Over Transition', *Adv. Mater.* **2017**, *29*, 1702257.
URL https://doi.org/10.1002/adma.201702257

[93] Hu, T.; Connor, A. L.; Miller, D. P.; Wang, X.; Pei, Q.; Liu, R.; He, L.; Zheng, C.; Zurek, E.; Lu, Z.-L.; Gong, B., 'Helical Folding of meta-Connected Aromatic Oligoureas', *Org. Lett.* **2017**, *19*, 2666–2669.
URL https://doi.org/10.1021/acs.orglett.7b01005

[92] Bi, T.; Miller, D. P.; Shamp, A.; Zurek, E., 'Superconducting Phases of Phosphorus Hydride Under Pressure: Stabilization by Mobile Molecular Hydrogen', *Angew. Chem. Int. Ed.* **2017**, *56*, 10192–10195.
URL https://doi.org/10.1002/ange.201701660

[91] Shamp, A.; Zurek, E.; Ogitsu, T.; Fratanduono, D. E.; Hamel, S., 'Properties of B_4C in the Shocked State for Pressures up to 1.5 TPa', *Phys. Rev. B* **2017**, *95*, 184111.
URL https://doi.org/10.1103/physrevb.95.184111

[90] Moustafa, S. G.; Schultz, A. J.; Zurek, E.; Kofke, D. A., 'Accurate and Precise ab initio Anharmonic Free-Energy Calculations for Metallic Crystals. Application to hcp Fe at High Temperature and Pressure', *Phys. Rev. B* **2017**, *96*, 014117.
URL http://doi.org/10.1103/PhysRevB.96.014117

[89] Avery, P.; Falls, Z.; Zurek, E., 'XtalOpt version r10: An Open-Source Evolutionary Algorithm for Crystal Structure Prediction', *Comput. Phys. Commun.* **2017**, *217*, 210–211.
URL https://doi.org/10.1016/j.cpc.2017.04.001

[88] Shamp, A.; Zurek, E., 'Superconductivity in Hydrides Doped with Main Group Elements Under Pressure', *Nov. Supercond. Mater.* **2017**, *3*, 14–22.
URL https://doi.org/10.1515/nsm-2017-0003

[87] Miller, D. P.; Hooper, J.; Simpson, S.; Costa, P. S.; Tyminska, N.; McDonnell, S. M.; Bennett, J. A.; Enders, A.; Zurek, E., 'Electronic Structure of Iron Porphyrin Adsorbed to the Pt(111) Surface', *J. Phys. Chem. C* **2016**, *120*, 29173–29181.
URL https://doi.org/10.1021/acs.jpcc.6b09408

[86] Avery, P.; Zurek, E., 'RandSpg: An Open-Source Program for Generating Atomistic Crystal Structures with Specific Spacegroups', *Comput. Phys. Commun.* **2017**, *213*, 208–216.
URL https://doi.org/10.1016/j.cpc.2016.12.005

[85] Beniwal, S.; Hooper, J.; Miller, D. P.; Costa, P.; Chen, G.; Liu, S.-Y.; Dowben, P. A.; Sykes, E. C. H.; Zurek, E.; Enders, A., 'Graphene-Like Boron-Carbon-Nitrogen Monolayers', *ACS Nano* **2017**, *11*, 2486–2493.
URL https://doi.org/10.1021/acsnano.6b08136

[84] Falls, Z.; Zurek, E.; J., A., 'Computational Prediction and Analysis of the ^{27}Al Solid-State NMR Spectrum of Methylaluminoxane (MAO) at Variable Temperatures and Field Strengths', *Phys. Chem. Chem. Phys.* **2016**, *18*, 24106–24118.
URL http://doi.org/10.1039/C6CP04260K

[83] Fratanduono, D. E.; Celliers, P. M.; Braun, D. G.; Sterne, P. A.; Hamel, S.; Shamp, A.; Zurek, E.; Wu, K. J.; Lazicki, A. E.; Millot, M.; Collins, G. W., 'Equation of State, Adiabatic Sound Speed and Gruneisen Coefficient of Boron Carbide Along the Principal Hugoniot to 700 GPa (7 Mbar)', *Phys. Rev. B.* **2016**, *94*, 184107.
URL https://doi.org/10.1103/PhysRevB.94.184107

[82] Zurek, E., 'Hydrides of the Alkali Metals and Alkaline Earth Metals Under Pressure', *Comments Inorg. Chem.* **2017**, *37*, 78–98.
URL https://doi.org/10.1080/02603594.2016.1196679

[81] Mounce, A.; Yasuoka, H.; Koutroulakis, G.; Lee, J. A.; Cho, H.; Gendron, F.; Zurek, E.; Scott, B. L.; Trujillo, J. A.; Slemmons, A. K.; Cross, J. N.; Thompson, J. D.; Kozimor, S. A.; Bauer, E. D.; Autschbach, J.; Clark, D. L., 'Nuclear Magnetic Resonance Measurements and Electronic Structure of Pu(IV) in $[Me_4N]_2PuCl_6$', *Inorg. Chem.* **2016**, *55*, 8371–8380.
URL https://doi.org/10.1021/acs.inorgchem.6b00735

[80] Zurek, E., 'The Pressing Role of Theory in Studies of Compressed Matter', in Dronskowski, R. (editor), 'Handbook of Solid State Chemistry', Vol. 5, Wiley-VCH Verlag GmbH & Co., Weinheim, Germany, **2017**, 571–605.
URL https://doi.org/10.1002/9783527691036.hsscvol5020

[79] Simpson, S.; Hooper, J.; Miller, D. P.; Kunkel, D. A.; Enders, E.; Zurek, E., 'Modulating Bond Lengths via Backdonation: A First-Principles Investigation of a Quinonoid Zwitterion Adsorbed to Coinage Metal Surfaces', *J. Phys. Chem. C* **2016**, *120*, 6633–6641.
URL https://doi.org/10.1021/acs.jpcc.6b00360

[78] Luo, X.; Zurek, E., 'Crystal Structures and Electronic Properties of Single-Layer, Few-Layer and Multilayer GeH', *J. Phys. Chem. C* **2016**, *120*, 793–800.
URL https://doi.org/10.1021/acs.jpcc.5b11770

[77] Murphy, C. J.; Miller, D. P.; Simpson, S.; Baggett, A.; Pronschinske, A.; Liriano, M. L.; Therrien, A. J.; Enders, A.; Liu, S.-Y.; Zurek, E.; Sykes, E. C. H., 'Charge-Transfer-Induced Magic Cluster Formation of Azaborine Heterocycles on Noble Metal Surfaces', *J. Phys. Chem. C* **2016**, *120*, 6020–6030.
URL https://doi.org/10.1021/acs.jpcc.5b11970

[76] Costa, P. S.; Miller, D. P.; Teeter, J. D.; Beniwal, S.; Zurek, E.; Sinitskii, A.; Hooper, J.; Enders, A., 'Structure and Proton-Transfer Mechanism in One-Dimensional Chains of Benzimidazoles', *J. Phys. Chem. C.* **2016**, *120*, 5804–5809.
URL https://doi.org/10.1021/acs.jpcc.6b00572

[75] Shamp, A.; Terpstra, T.; Bi, T.; Falls, Z.; Avery, P.; Zurek, E., 'Decomposition Products of Phosphine Under Pressure: PH_2 Stable and Superconducting?', *J. Am. Chem. Soc.* **2016**, *138*, 1884–1892.
URL https://doi.org/10.1021/jacs.5b10180

[74] Zhang, R. F.; Wen, X. D.; Legut, D.; Fu, Z. H.; Veprek, S.; Zurek, E.; Mao, H. K., 'Crystal Field Splitting is Limiting the Stability and Strength of Ultra-Incompressible Orthorhombic Transition Metal Tetraborides', *Sci. Rep.* **2016**, *6*, 23088.
URL https://doi.org/10.1038/srep23088

[73] Falls, Z.; Lonie, D. C.; Avery, P.; Shamp, A.; Zurek, E., 'XtalOpt Version r9: An Open-Source Evolutionary Algorithm for Crystal Structure Prediction', *Comput. Phys. Commun.* **2016**, *199*, 178–179.
URL https://doi.org/10.1016/j.cpc.2015.09.018

[72] Miao, M.-S.; Botana, J.; Zurek, E.; Hu, T.; Liu, J.; Yang, W., 'Electron Counting and a Large Family of Two-Dimensional Semiconductors', *Chem. Mater.* **2016**, *28*, 1994–1999.
URL https://doi.org/10.1021/acs.chemmater.5b03557

[71] Kunkel, D. A.; Hooper, J.; Bradley, B.; Schleuter, L.; Rasmussen, T.; Costa, P.; Beniwal, S.; Ducharme, S.; Zurek, E.; Enders, A., '2D Co-Crystallization from H-Bonded Organic Ferroelectrics', *J. Phys. Chem. Lett.* **2016**, *7*, 435–440.
URL http://doi.org/10.1021/acs.jpclett.5b02472

[70] Terpstra, T.; Hooper, J.; Zurek, E., 'First Principles Investigation on How Site Preference and Entropy Affects the Stability of $(Eu_xM_{1-x})_2Ge_2Pb$ (M = Ca, Sr, Ba) Polar Intermetallics', *Can. J. Chem.* **2016**, *94*, 312–320.
URL https://doi.org/10.1139/cjc-2015-0374

[69] Shamp, A.; Zurek, E., 'Superconducting High-Pressure Phases Composed of Hydrogen and Iodine', *J. Phys. Chem. Lett.* **2015**, *6*, 4067–4072.
URL https://doi.org/10.1021/acs.jpclett.5b01839

[68] Hooper, J.; Kunkel, D. A.; Zurek, E.; Enders, A., 'Interplay Between Hydrogen Bonding, Epitaxy, and Charge Transfer in the Self-Assembly of Croconic Acid on Au(111) and Ag(111)', *J. Phys. Chem. C* **2015**, *119*, 26429–26437.
URL https://doi.org/10.1021/acs.jpcc.5b06589

[67] Tymińska, N.; Zurek, E., 'DFT-D Investigation of Active and Dormant Methylaluminoxane (MAO) Species Grafted onto a Magnesium Dichloride Cluster: A Model Study of Supported MAO', *ACS Catal.* **2015**, *5*, 6989–6998.
URL https://doi.org/10.1021/acscatal.5b01697

[66] Shamp, A.; Saitta, P.; Zurek, E., 'Theoretical Predictions of Novel Potassium Chloride Phases Under Pressure', *Phys. Chem. Chem. Phys.* **2015**, *17*, 12265–12272.
URL https://doi.org/10.1039/c5cp00470e

[65] Zurek, E.; Yao, Y., 'Theoretical Predictions of Novel Superconducting Phases of $BaGe_3$ Stable at Atmospheric and High Pressures', *Inorg. Chem.* **2015**, *54*, 2875–2884.
URL https://doi.org/10.1021/ic5030235

[64] Murphy, C. J.; Baggett, A. W.; Miller, D. P.; Simpson, S.; Marcinkowski, M. D.; Mattera, M. F. G.; Pronschinske, A.; Therrien, A.; Liriano, M. L.; Zurek, E.; Liu, S.-Y.; Sykes, E. C. H., 'Effect of BN/CC Isosterism on the Thermodynamics of Surface and Bulk Binding: 1,2-Dihydro-1,2-azaborine vs. Benzene', *J. Chem. Phys.* **2015**, *119*, 14624–14631.
URL http://doi.org/10.1021/jp5126427

[63] Kunkel, D. A.; Hooper, J.; Simpson, S.; Miller, D. P.; Routaboul, L.; Braunstein, P.; Doudin, B.; Beniwal, S.; Dowben, P.; Skomski, R.; Zurek, E.; Enders, A., 'Self-Assembly of Strongly Dipolar Molecules on Metal Surfaces', *J. Chem. Phys.* **2015**, *142*, 101921 (1–9).
URL https://doi.org/10.1063/1.4907943

[62] Miller, D. P.; Simpson, S.; Tyminska, N.; Zurek, E., 'Benzene Derivatives Adsorbed to the Ag(111) Surface: Binding Sites and Electronic Structure', *J. Chem. Phys.* **2015**, *142*, 101924 (1–13).
URL https://doi.org/10.1063/1.4908267

[61] Zurek, E.; Grochala, W., 'Predicting Crystal Structures and Properties of Matter Under Extreme Conditions via Quantum Mechanics: the Pressure is On', *Phys. Chem. Chem. Phys.* **2015**, *17*, 2917–2934.
URL http://doi.org/10.1039/c4cp04445b

[60] Falls, Z.; Tyminska, N.; Zurek, E., 'The Dynamic Equilibrium Between $(AlOMe)_n$ Cages and $(AlOMe)_n \cdot (AlMe_3)_m$ Nanotubes in Methylaluminoxane (MAO): A First-Principles Investigation', *Macromolecules* **2014**, *47*, 8556–8569.
URL http://doi.org/10.1021/ma501892v

[59] Dannenhoffer, A.; Baker, J.; Pantano, N.; Stachowski, J.; Zemla, D.; Swanson, W.; Zurek, E.; Szczepankiewicz, S.; Kozik, M., 'Dimerization of Cobalt-Substituted Keggin Phosphotungstate, $[PW_{11}O_{39}Co(X)]^{5-}$, in Nonpolar Solvents', *J. Coord. Chem.* **2014**, *67*, 2830–2842.
URL http://doi.org/10.1080/00958972.2014.956664

[58] Simpson, S.; Gross, M. S.; Olson, J. R.; Zurek, E.; Aga, D. S., 'Identification of Polybrominated Diphenyl Ether Metabolites Based on Calculated Boiling Points from COSMO-RS, Experimental Retention Times, and Mass Spectral Fragmentation Patterns', *Anal. Chem.* **2015**, *87*, 2299–2305.
URL http://doi.org/10.1021/ac504107b

[57] Beniwal, S.; Chen, S.; Kunkel, D. A.; Hooper, J.; Simpson, S.; Zurek, E.; Zeng, X. C.; Enders, A., 'Kagome-Like Lattice of π-π Stacked 3-Hydroxyphenalenone on Cu(111)', *Chem. Commun.* **2014**, *50*, 8659–8662.
URL http://doi.org/10.1039/c4cc03523b

[56] Zurek, E., 'Discovering New Materials via *a priori* Crystal Structure Prediction', in Parrill, A. L.; Lipkowitz, K. B. (editors), 'Reviews in computational chemistry', Vol. 29, John Wiley & Sons, Inc., Hoboken, New Jersey, **2016**, 274–326.
URL https://doi.org/10.1002/9781119148739.ch5

[55] Seel, A. G.; Zurek, E.; Ramirez-Cuesta, A. J.; Ryan, K. R.; Lodge, M. T. J.; Edwards, P. P., 'Low Energy Structural Dynamics and Constrained Libration of $Li(NH_3)_4$, the Lowest Melting Point Metal', *Chem. Commun.* **2014**, *50*, 10778–10781.
URL http://doi.org/10.1039/c4cc03397c

[54] Bovino, M. T.; Liwosz, T. W.; Kendel, N. E.; Miller, Y.; Tyminska, N.; Zurek, E.; Chemler, S. R., 'Enantioselective Copper-Catalyzed Carboetherification of Unactivated Alkenes', *Angew. Chem. Int. Ed.* **2014**, *53*, 6383–6387.
URL http://doi.org/10.1002/anie.201402462

[53] Hooper, J.; Kunkel, D. A.; Simpson, S.; Beniwal, S.; Enders, A.; Zurek, E., 'Chiral Surface Networks of 3-HPLN - A Molecular Analog of Rounded Triangle Assembly', *Surf. Sci.* **2014**, *629*, 65–74.
URL https://doi.org/10.1016/j.susc.2014.04.015

[52] Hooper, J.; Terpstra, T.; Shamp, A.; Zurek, E., 'Composition and Constitution of Compressed Strontium Polyhydrides', *J. Phys. Chem. C* **2014**, *118*, 6433–6447.
URL https://doi.org/10.1021/jp4125342

[51] Kunkel, D. A.; Hooper, J.; Simpson, S.; Beniwal, S.; Morrow, K. L.; Smith, D. C.; Cousins, K.; Ducharme, S.; Zurek, E.; Enders, A., 'Rhodizonic Acid on Noble Metals: Surface Reactivity and Coordination Chemistry', *J. Phys. Chem. Lett.* **2013**, *4*, 3413–3419.
URL http://doi.org/10.1021/jz4016124

[50] Pritchard, B. P.; Simpson, S.; Zurek, E.; Autschbach, J., 'Computation of Chemical Shifts for Paramagnetic Molecules: A Laboratory Experiment for the Undergraduate Curriculum', *J. Chem. Educ.* **2014**, *91*, 1058–1063.
URL https://doi.org/10.1021/ed400902c

[49] Simpson, S.; van Fleet, A.; Zurek, E., 'A Computational Investigation of a Molecular Switch', *J. Chem. Educ.* **2013**, *90*, 1528–1532.
URL https://doi.org/10.1021/ed400278x

[48] Wach, A.; Chen, J.; Falls, Z.; Lonie, D.; Mojica, E.-R.; Aga, D.; Autschbach, J.; Zurek, E., 'Determination of the Structures of Molecularly Imprinted Polymers and Xerogels Using an Automated Stochastic Approach', *Anal. Chem.* **2013**, *85*, 8577–8584.
URL https://doi.org/10.1021/ac402004z

[47] Simpson, S.; Kunkel, D. A.; Hooper, J.; Nitz, J.; Dowben, P. A.; Routaboul, L.; Braunstein, P.; Doudin, B.; Enders, A.; Zurek, E., 'Coverage-Dependent Interactions at the Organics-Metal Interface: Quinonoid Zwitterions on Au(111)', *J. Phys. Chem. C* **2013**, *117*, 16406–16415.
URL https://doi.org/10.1021/jp403384h

[46] Hooper, J.; Altintas, B.; Shamp, A.; Zurek, E., 'Polyhydrides of the Alkaline Earth Metals: A Look at the Extremes Under Pressure', *J. Phys. Chem. C* **2013**, *117*, 2982–2992.
URL https://doi.org/10.1021/jp311571n

[45] Lonie, D. C.; Hooper, J.; Altintas, B.; Zurek, E., 'Metallization of Magnesium Polyhydrides Under Pressure', *Phys. Rev. B* **2013**, *87*, 054107 (1–8).
URL https://doi.org/10.1103/physrevb.87.054107

[44] Simpson, S.; Autschbach, J.; Zurek, E., 'Computational Modeling of the Optical Rotation of Amino Acids: An 'in silico' Experiment for Physical Chemistry', *J. Chem. Educ.* **2013**, *90*, 656–660.
URL http://doi.org/10.1021/ed300680g

[43] Simpson, S.; Lonie, D. C.; Chen, J.; Zurek, E., 'A Computational Experiment on Single-Walled Carbon Nanotubes', *J. Chem. Educ.* **2013**, *90*, 651–655.
URL https://doi.org/10.1021/ed3006067

[42] Kunkel, D. A.; Hooper, J.; Simpson, S.; Rojas, G. A.; Ducharme, S.; Usher, T.; Zurek, E.; Enders, A., 'Proton Transfer in Surface-Stabilized Chiral Motifs of Croconic Acid', *Phys. Rev. B* **2013**, *87*, 041402(R) (1–4).
URL http://doi.org/10.1103/PhysRevB.87.041402

[41] Hanwell, M. D.; Curtis, D. E.; Lonie, D. C.; Vandermeersch, T.; Zurek, E.; Hutchison, G. R., 'Avogadro: An Advanced Semantic Chemical Editor, Visualization, and Analysis Platform', *J. Cheminf.* **2012**, *4*, 17 (1–17).
URL https://doi.org/10.1186/1758-2946-4-17

[40] Jewell, A. D.; Simpson, S. M.; Enders, A.; Zurek, E.; Sykes, E. C. H., 'Magic Electret Clusters of 4-Fluorostyrene on Metal Surfaces', *J. Phys. Chem. Lett.* **2012**, *3*, 2069–2075.
URL https://doi.org/10.1021/jz3006783

[39] Shamp, A.; Hooper, J.; Zurek, E., 'Compressed Cesium Polyhydrides: Cs^+ Sublattices and H_3^- Three-Connected Nets', *Inorg. Chem.* **2012**, *51*, 9333–9342.
URL http://doi.org/10.1021/ic301045v

[38] Suen, N.-T.; Hooper, J.; Zurek, E.; Bobev, S., 'On the Nature of Ge-Pb Bonding in the Solid State. Synthesis, Structural Characterization, and Electronic Structures of Two Unprecedented Germanide-Plumbides', *J. Am. Chem. Soc.* **2012**, *134*, 12708–12716.
URL http://doi.org/10.1021/ja3042838

[37] Simpson, S.; Zurek, E., 'Substituted Benzene Derivatives on the Cu(111) Surface', *J. Phys. Chem. C* **2012**, *116*, 12636–12643.
URL https://doi.org/10.1021/jp302682n

[36] Kunkel, D. A.; Simpson, S.; Nitz, J.; Rojas, G. A.; Zurek, E.; Routaboul, L.; Doudin, B.; Braunstein, P.; Dowben, P. A.; Eders, A., 'Dipole Driven Bonding Schemes of Quinoid Zwitterions on Surfaces', *Chem. Commun.* **2012**, *48*, 7143–7145.
URL https://doi.org/10.1039/c2cc32462h

[35] Hooper, J.; Zurek, E., 'High Pressure Potassium Polyhydrides: A Chemical Perspective', *J. Phys. Chem. C* **2012**, *116*, 13322–13328.
URL https://doi.org/10.1021/jp303024h

[34] Hooper, J.; Zurek, E., 'Lithium Subhydrides Under Pressure and their Superatom–Like Building Blocks', *ChemPlusChem* **2012**, *77*, 969–972.
URL https://doi.org/10.1002/cplu.201200130

[33] Lonie, D. C.; Zurek, E., 'Identifying Duplicate Crystal Structures: XtalComp, an Open–Source Solution', *Comput. Phys. Commun.* **2012**, *183*, 690–697.
URL https://doi.org/doi:10.1016/j.cpc.2011.11.007

[32] Hooper, J.; Zurek, E., 'Rubidium Polyhydrides Under Pressure: Emergence of the Linear H_3^- Species', *Chem. Eur. J.* **2012**, *18*, 5013–5021.
URL https://doi.org/10.1002/chem.201103205

[31] Rojas, G.; Simpson, S.; Chen, X.; Kunkel, D. A.; Nitz, J.; Xiao, J.; Dowben, P. A.; Zurek, E.; Enders, A., 'Surface State Engineering of Molecule-Molecule Interactions', *Phys. Chem. Chem. Phys.* **2012**, *14*, 4971–4976.
URL https://doi.org/10.1039/c2cp40254h

[30] Lonie, D. C.; Zurek, E., 'XtalOpt version r7: An Open-Source Evolutionary Algorithm for Crystal Structure Prediction', *Comput. Phys. Commun.* **2011**, *182*, 2305–2306.
URL https://doi.org/10.1016/j.cpc.2011.06.003

[29] Hooper, J.; Baettig, P.; Zurek, E., 'Pressure Induced Structural Transitions in KH, RbH and CsH', *J. Appl. Phys.* **2012**, *111*, 112611.
URL https://doi.org/10.1063/1.4726210

[28] Baettig, P.; Zurek, E., 'Pressure-Stabilized Sodium Polyhydrides, NaH_n ($n > 1$)', *Phys. Rev. Lett.* **2011**, *106*, 237002 (1–4).
URL https://doi.org/10.1103/physrevlett.106.237002

[27] Zurek, E., 'Alkali Metals in Ethylenediamine: A Computational Study of the Optical Absorption Spectra and NMR Parameters of $[M(en)_3^+ \cdot M^-]$ Ion-Pairs', *J. Am. Chem. Soc.* **2011**, *133*, 4829–4839.
URL https://doi.org/10.1021/ja1085244

[26] Zurek, E.; Wen, X.-D.; Hoffmann, R., '(Barely) Solid $Li(NH_3)_4$: The Electronics of an Expanded Metal', *J. Am. Chem. Soc.* **2011**, *133*, 3535–3547.
URL https://doi.org/10.1021/ja109397k

[25] Lonie, D. C.; Zurek, E., 'XtalOpt: An Open-Source Evolutionary Algorithm for Crystal Structure Prediction', *Comput. Phys. Commun.* **2011**, *182*, 372–387.
URL https://doi.org/10.1016/j.cpc.2010.07.048

[24] Zurek, E.; Autschbach, J., 'Ab-Initio NMR Computations for Carbon Nanotubes', in Nalwa, H. S. (editor), 'Encyclopedia of Nanoscience and Nanotechnology', Vol. 11, American Scientific Publishers, Stevenson Ranch, CA, 2nd edition, **2011**, 59–73.
URL http://www.aspbs.com/enn.html

[23] Zurek, E.; Jepsen, O.; Andersen, O. K., 'Searching for the Interlayer Band and Unravelling the Bonding in β-$ThSi_2$ and α-$ThSi_2$ with *N*MTO Wannier-like Functions', *Inorg. Chem.* **2010**, *49*, 1384–1396.
URL https://doi.org/10.1021/ic9014515

[22] Zurek, E.; Autschbach, J., 'NMR Computations for Carbon Nanotubes from First Principles: Present Status and Future Directions', *Int. J. Quantum Chem.* **2009**, *109*, 3343–3367.
URL https://doi.org/10.1002/qua.22211

[21] Zurek, E.; Hoffmann, R.; Ashcroft, N. W.; Oganov, A. R.; Lyakhov, A. O., 'A Little Bit of Lithium Does a Lot for Hydrogen', *Proc. Natl. Acad. Sci. U.S.A.* **2009**, *106*, 17640–17643.
URL https://doi.org/10.1073/pnas.0908262106

[20] Zurek, E.; Edwards, P. P.; Hoffmann, R., 'A Molecular Perspective on Lithium-Ammonia Solutions', *Angew. Chem. Int. Ed.* **2009**, *48*, 8198–8232.
URL https://doi.org/10.1002/anie.200900373

[19] Zurek, E.; Pickard, C. J.; Autschbach, J., 'A Density Functional Studies of the ^{13}C NMR Chemical Shifts of Fluorinated Single–Walled Carbon Nanotubes', *J. Phys. Chem. A* **2009**, *113*, 4117–4124.
URL http://doi.org/10.1021/jp810523x

[18] Zurek, E.; Pickard, C. J.; Autschbach, J., 'Density Functional Study of the ^{13}C NMR Chemical Shifts in Single-Walled Carbon Nanotubes with Stone–Wales Defects', *J. Phys. Chem. C* **2008**, *112*, 11744–11750.
URL http://doi.org/10.1021/jp803180v

[17] Zurek, E.; Autschbach, J.; Malinowski, N.; Enders, A.; Kern, K., 'Experimental and Theoretical Investigations of the Thermodynamic Stability of Ba–C_{60} and K–C_{60} Clusters', *ACS Nano* **2008**, *2*, 1000–1014.
URL http://doi.org/10.1021/nn800022d

[16] Zurek, E.; Pickard, C. J.; Autschbach, J., 'Determining the Diameter of Functionalized Single-Walled Carbon Nanotubes using ^{13}C NMR: A Theoretical Study', *J. Phys. Chem. C* **2008**, *112*, 9267–9271.
URL https://doi.org/10.1021/jp800873c

[15] Zurek, E.; Autschbach, J.; Andersen, O. K., 'Downfolding and *N*-ization of a Basis Set of Slater Type Orbitals', in Simos, T. E.; Maroulis, G. (editors), 'Computation in Modern Science and Engineering Proceedings of the International Conference on Computational Methods in Science and Engineering 2007', Number volume 2, part B in Conference Proceedings 963, American Institue of Physics, **2007**, 1421–1424.
URL https://doi.org/10.1063/1.2836021

[14] Zurek, E.; Autschbach, J., 'Density Functional Studies of the ^{13}C NMR Chemical Shifts in Single–Walled Carbon Nanotubes', in Simos, T. E.; Maroulis, G. (editors), 'Computation in Modern Science and Engineering Proceedings of the International Conference on Computational Methods in Science and Engineering 2007', Number volume 2, part B in Conference Proceedings 963, American Institue of Physics, **2007**, 1425–1428.
URL https://doi.org/10.1063/1.2836022

[13] Zurek, E.; Pickard, C. J.; Autschbach, J., 'A Density Functional Study of the ^{13}C NMR Chemical Shifts in Functionalized Single–Walled Carbon Nanotubes', *J. Am. Chem. Soc.* **2007**, *129*, 4430–4439.
URL http://doi.org/10.1021/ja069110h

[12] Enders, A.; Malinowski, N.; Ievlev, D.; Zurek, E.; Autschbach, J.; Kern, K., 'Magic Alkali-fullerene Compound Clusters of Extreme Thermal Stability', *J. Chem. Phys.* **2006**, *125*, 191102–(1–4).
URL http://doi.org/10.1063/1.2400027

[11] Zurek, E.; Pickard, C. J.; Walczak, B.; Autschbach, J., 'Density Functional Calculations of the ^{13}C NMR Chemical Shifts in Small-to-Medium-Diameter Infinite Single-Walled Carbon nanotube', *J. Phys. Chem. A* **2006**, *110*, 11995–12004.
URL http://doi.org/10.1021/jp064540f

[10] Zurek, E.; Jepsen, O.; Andersen, O. K., 'Muffin-Tin Orbital Wannier-Like Functions for Insulators and Metals', *ChemPhysChem* **2005**, *6*, 1934–1942.
URL http://doi.org/10.1002/cphc.200500133

[9] Zurek, E.; Autschbach, J., 'Density Functional Calculations of the ^{13}C NMR Chemical Shifts in (9,0) Single-Walled Carbon Nanotubes', *J. Am. Chem. Soc.* **2004**, *126*, 13079–13088.
URL http://doi.org/10.1021/ja047941m

[8] Zurek, E.; Ziegler, T., 'Theoretical Studies of the Structure and Function of MAO (Methylaluminoxane)', *Prog. Polym. Sci.* **2004**, *29*, 107–148.
URL http://doi.org/10.1016/j.progpolymsci.2003.10.003

[7] Autschbach, J.; Zurek, E., 'Relativistic Density-Functional Computations of the Chemical Shift of ^{129}Xe in Xe@C_{60}', *J. Phys. Chem. A* **2003**, *107*, 4967–4972.
URL http://doi.org/10.1021/jp0346559

[6] Zurek, E.; Ziegler, T., 'A Theoretical Study of the Insertion Barrier of MAO (methylaluminoxane)-Activated, Cp_2ZrMe_2-Catalyzed Ethylene Polymerization: Further Evidence for the Structural Assignment of Active and Dormant Species.', *Faraday Discuss.* **2003**, *124*, 93–109.
URL https://doi.org/10.1039/B209455J

[5] Xu, Z.; Vanka, K.; Firman, T.; Michalak, A.; Zurek, E.; Zhu, C.; Ziegler, T., 'Theoretical Study of the Interactions between Cations and Anions in Group IV Transition-Metal Catalysts for Single-Site Homogeneous Olefin Polymerization.', *Organometallics* **2002**, *21*, 2444–2453.
URL http://doi.org/10.1021/om011057c

[4] Zurek, E.; Ziegler, T., 'Toward the Identification of Dormant and Active Species in MAO (Methylaluminoxane)-Activated, Dimethylzirconocene-Catalyzed Olefin Polymerization.', *Organometallics* **2002**, *21*, 83–92.
URL http://doi.org/10.1021/om010812j

[3] Zurek, E.; Woo, T. K.; Firman, T. K.; Ziegler, T., 'Modeling MAO (Methylaluminoxane)', in Blom, R.; Follestad, A.; Rytter, E.; Tilset, M.; Ystenes, M. (editors), 'Organometallic Catalysts and Olefin Polymerization: Catalysts for a New Millenium', Springer, Berlin, Heidelberg, **2001**, 109–123.
URL https://doi.org/10.1007/978-3-642-59465-6_10

[2] Zurek, E.; Ziegler, T., 'A Combined Quantum Mechanical and Statistical Mechanical Study of the Equilibrium of Trimethylaluminum (TMA) and Oligomers of $(AlOCH_3)_n$ Found in Methylaluminoxane (MAO).', *Inorg. Chem.* **2001**, *40*, 3279–3292.
URL http://doi.org/10.1021/ic001444z

[1] Zurek, E.; Woo, T. K.; Firman, T. K.; Ziegler, T., 'Modeling the Dynamic Equilibrium Between Oligomers of $(AlOCH_3)_n$ in Methylaluminoxane (MAO). A Theoretical Study Based on a Combined Quantum Mechanical and Statistical Mechanical Approach.', *Inorg. Chem.* **2001**, *40*, 361–370.
URL http://doi.org/10.1021/ic000845b

Invited Conference Talks, Workshops & Seminars

Upcoming

- National Ignition Facility and Jupiter Laser Facility User Group Meeting; Livermore; Jan 2024.
- Distinguished Lectures in Quantum Crystallography and Related Fields; Virtual; Feb 2024.
- ECLIPSE Meeting; Rochester; April 2024.
- Discussion Leader, Gordon Research Conference on Research at High Pressure; Holderness School; July 2024.
- Canadian Symposium on Theoretical and Computational Chemistry; Halifax, Canada; July 2024.
- CBOND2024: The 3rd European Symposium on Chemical Bonding; Amsterdam; Sept 2024.

Conferences, Workshops, Summer Schools

March 2020 - March 2022 virtual format; else in-person unless otherwise stated.

74. "Future Directions in Structure Prediction" & Tutorial on XtalOpt, 8th Annual JHU Summer School; Data Driven Materials Discovery: From ML to Maker Space, John Hopkins University; Aug 2023.

73. "Extreme Chemistry and New States of Matter at Extreme Pressures", 28th AIRAPT and 60th EHPRG high-pressure conference, Edinburgh, Plenary; July 2023.

72. "Theoretical Design of Light Element Superconductors", North Eastern Regional ACS Meeting, Boston; June 2023.

71. "Exotic Chemistry and New States of Matter at Extreme Pressures", Center for Matter at Atomic Pressures Undergraduate Summer School, University of Rochester; June 2023 (virtual participation).

70. "Theoretical Design of Light Element Superconductors", Gordon Research Conference on Superconductivity; Les Diablerets, Switzerland; May 2023.

69. "The XtalOpt Evolutionary Algorithm for Crystal Structure Prediction", American Physical Society March Meeting; Las Vegas; March 2023.

68. “Theoretical Design of Light Element Superconductors”, 2022 IUCr High-Pressure Workshop, Argonne National Lab; Dec 2022 (virtual participation).

67. “Theoretical Design of Light Element Superconductors”, Frontiers of High Pressure Research – Science under Extreme Conditions (Nature Conferences), Shanghai, China; Nov 2022 (virtual participation).

66. “Exotic Chemistry and New States of Matter at Extreme Pressures”, Center for Matter at Atomic Pressures Undergraduate Summer School, University of Rochester; Aug 2022 (virtual participation).

65. “Theoretical Design of Light Element Superconductors”, 33rd IUPAP Conference on Computational Physics (CCP 2020); Austin, Texas; Aug 2022 (virtual participation).

64. “Ternary Hydride Superconductors Under Pressure”, International Workshop on Challenges in Designing Room Temperature Superconductors, L’Aquila, Italy; July 2022 (virtual participation).

63. “Theoretical Predictions of Superhard and Superconducting Carbon Polymorphs”, International Symposium on Theoretical and Computational Materials Science; Jilin, China; July 2022 (virtual participation).

62. “Putting the Squeeze on Matter”, Exploring High Pressure Science at the Extremes Through Experiment and Computation, Gordon Research Conference; Holderness School; July 2022.

61. “Towards Room-Temperature Superconductivity in Doped H_3S Phases Under Pressure?”, 12th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), Vancouver, Canada; July 2022.

60. “Theoretical Design of Light Element Superconductors”, 10th Triennial Conference on Molecular Quantum Mechanics, Blacksburg, Virgina; June 2022.

59. “The XtalOpt Evolutionary Algorithm for Crystal Structure Prediction”, International School of Crystallography, Erice, Italy; workshop presentation; June 2022.

58. “Crystal Structure Prediction”, International School of Crystallography, Erice, Italy; June 2022.

57. “Superconducting High Pressure Hydrides”, International School of Crystallography, Erice, Italy; June 2022.

56. “Theoretical Predictions of Superconducting Materials Under Pressure”, Next-Generation Materials Structure-Property Prediction, Pacifichem; Honolulu, Hawaii; December 2021.

55. “Towards Room Temperature Superconductivity in Hydride-Based Materials Under Pressure?”, 10th Asian Conference on High Pressure Research; Seoul, Korea; October 2021.

54. “The XtalOpt Evolutionary Algorithm for Crystal Structure Prediction”, Computational Methods in Materials Science, Fundamentals and Applications; EMRS - Warsaw; workshop presentation; Sept 2021.

53. “Theoretical Predictions of Superconducting and Superhard Materials”, European Materials Research Society (EMRS), Warsaw, Poland; Sept 2021.

52. “Exotic Chemistry and New States of Matter at Extreme Pressures”, Center for Matter at Atomic Pressures Undergraduate Summer School, University of Rochester; Aug 2021.

51. “Theoretical Predictions of Superconducting and Superhard Materials”, Chemistry at Extremes Workshop, Oak Ridge National Laboratory; Aug 2021.

50. “Predicting Superhard Materials via a Machine-Learning-Informed Evolutionary Structure Search”, Telluride Workshop on Computational Materials Chemistry, Telluride, Colorado; July 2021.

49. “Theoretical Predictions of Light and Warm Superconductors”, American Physical Society; March 2021.

48. “Electronic Structure and Superconductivity in Compressed Binary and Ternary Hydrides”, European High Pressure Research Group International Conference; Tenerife, Spain; plenary; Sept 2020.

47. “Theoretical Predictions of Superconducting and Superhard Materials”, 100 years Polish Chemical Society; Warsaw, Poland; Sept 2019.

46. “Theoretical Predictions of Superconducting and Superhard Materials”, International Union of Crystallography, high pressure workshop; Vienna, Austria; plenary; Aug 2019.
45. “Chemistry Under Pressure”, Eric Pitman Summer Workshop in Computational Science, Center for Computational Research, Buffalo; July 2019.
44. “Theoretical Predictions of Unique Hydride Phases Under Pressure”, Understanding the Interaction of Hydrogen with Materials, Gordon Research Conference; Barcelona, Spain; June 2019.
43. “Computational Discovery of Novel Superconducting Phases Under Pressure”, SMEC2019; April 2019.
42. “Predicting Superhard Materials via a Machine-Learning-Informed Evolutionary Structure Search”, Study of Matter at Extreme Conditions 2019 (SMEC2019), an international conference hosted by the High Pressure Science Society of North America (HiPSSA); held on the *Celebrity Equinox*; April 2019.
41. “Computational Discovery of New Materials Under Pressure”, XXX IUPAP Conference on Computational Physics, University of California, Davis; July, 2018.
40. “Theoretical Predictions of Unique Hydride Phases Under Pressure”, Atoms, Molecules and Materials in Extreme Environments, Oslo, Norway; June, 2018.
39. “Chemistry Under Pressure”, Eric Pitman Summer Workshop in Computational Science, Center for Computational Research, Buffalo; July 2018.
38. “Chemistry Under Pressure”, 16th International Congress of Quantum Chemistry, Menton, France; June, 2018.
37. “Chemistry Under Pressure”, Molecular Education and Research Consortium in Undergraduate computational chemistRY (MERCURY); Furman University, South Carolina; July 2017.
36. “DFT Studies of B_4C Under Static and Dynamic Compression for up to 1.5 TPa”, 6th International Conference on Chemical Bonding; Hawaii; June 2017.
35. “DFT Studies of B_4C Under Static and Dynamic Compression for up to 1.5 TPa”, Equation-of-States Workshop, Laboratory for Laser Energetics, University of Rochester; May 2017.
34. “Computational Discovery of Materials Under Pressure”, American Physical Society; New Orleans; March 2017.
33. “Materials from First Principles”, Energy and Sustainable Materials Workshop, University of Oregon; Oct 2016.
32. “Theoretical Predictions of (Superconducting) Hydrides under Pressure”, North East Regional Meeting of the ACS, Binghamton; Oct 2016.
31. “Theoretical Predictions of (Superconducting) Hydrides under Pressure”, Theory and Applications of Computational Chemistry (TACC 2016); Seattle, Washington; Sept 2016.
30. “Superconductivity in High Pressure Hydrides”, International Conference on High Pressure in Semiconductor Physics (HPSP-17) & Workshop on High-pressure Study on Superconductors (WHS); Tokyo, Japan; Aug 2016.
29. “Theoretical Predictions of Hydrides with Novel Stoichiometries”, Solid State Chemistry Gordon Research Conference; Colby Sawyer College; July 2016.
28. “Structure Prediction Under Pressure”, 62nd American Vacuum Society International Symposium, “Accelerating Materials Discovery for Global Competitiveness” Session; San Jose; Oct 2015.
27. “Chemical Structure and Bonding Under Pressure”, 3rd International Conference on Chemical Bonding; Hawaii; July 2015.
26. “Structure Prediction Under Pressure”, Telluride Workshop on Computational Materials Chemistry; Colorado; June 2015.
25. “Chemistry Under Pressure”, North American Solid State Chemistry Conference; Tallahassee; June 2015.
24. “Bonding at the Metal-Organic Interface”, American Physical Society Meeting; San Antonio; March 2015.

23. “Structure Prediction from First Principles”, Quantum Systems in Chemistry, Physics and Biology; Taipei, Taiwan; Oct 2014.
22. “Building a Chemical Intuition Under Pressure”, American Chemical Society, San Francisco; Aug 2014.
21. “Building a Chemical Intuition Under Pressure: Prediction of Novel Hydrides”, Tuning Energy Density to Reveal or Control Properties of Extreme Matter, Gordon Conference; University of New England; June 2014.
20. “A Molecular Orbital Analysis of Electron Solvation”, Colloque Davy-Weyl: Electron solvation and electron transfer; Kavli Meeting, Buckinghamshire, UK; May 2014.
19. “Structure Prediction from First Principles”, The Minerals, Metals and Materials Society Meeting; San Diego; Feb 2014.
18. “Structure Prediction from First Principles Calculations”, WoPhys 2013 (MRSEC/CNFM Conference for Undergraduate Women in Physical Sciences), University of Nebraska-Lincoln; Oct 2013.
17. “Boron Carbide Under Extreme Conditions”, Carnegie/DOE Alliance Center Workshop; Chicago; Sept 2013.
16. “Building a Chemical Intuition Under Pressure: Predictions of Novel Hydrides”, 6th CTTC Theoretical Chemistry Conference; Krakow, Poland; Sept 2013.
15. “Building a Chemical Intuition Under Pressure: Prediction of Alkali Metal Polyhydrides and Subhydrides”, International Conference on High Pressure Science and Technology (AIRAPT); Seattle; July 2013.
14. “Predicting Potential Superconductors Under Pressure”, SMEC2013; March 2013.
13. “Building a Chemical Intuition Under Pressure: Compressed Polyhydrides and Subhydrides”, Study of Matter at Extreme Conditions 2013 (SMEC2013), an international conference hosted by the High Pressure Science Society of North America (HiPSSA); held on the *Celebrity Reflection*; March 2013.
12. “Developing a Chemical Intuition Under Pressure”, 2012 — Exploring Giant Planets on NIF (National Ignition Facility): A New Generation of Condensed Matter; Lawrence Livermore National Laboratory (LLNL); Dec 2012.
11. “Role of the Support in MAO (methylaluminoxane) Activated Olefin Polymerization”, North East Regional Meeting of the ACS; Rochester; Sept 2012.
10. “Locating the (Global and Local) Minima of Clusters and Solids”; LLNL; 2012 Computational Chemistry and Materials Science Summer Institute (CCMS); June 2012.
9. “Chemistry under High Pressure: Building a Chemical Intuition via Crystal Structure Prediction”, LLNL; CCMS; June 2012.
8. “Building a Chemical Intuition Under Pressure: Prediction of Alkali Metal Polyhydrides and Subhydrides”, 95^{th} Canadian Chemistry Conference and Exhibition (CSC 2012); Calgary, Canada; May 2012.
7. “Pressure Stabilized Alkali Metal Polyhydrides”, The Minerals, Metals and Materials Society Meeting; Orlando; March 2012.
6. “Chemistry Under Extreme Pressures — A Return to Simplicity?”, 2011 — Exploring Giant Planets on NIF (National Ignition Facility): A New Generation of Condensed Matter Workshop; LLNL; Dec 2011.
5. “Pressure Stabilized Alkali Metal Polyhydrides”, International Conference on High Pressure Science and Technology (AIRAPT); Mumbai, India; Sept 2011.
4. “Theoretical Predictions of Pressure–Stabilized Alkali Metal Polyhydrides”, SMEC2011; March 2011.
3. “Solid $Li(NH_3)_4$: An Expanded Metal Under Pressure”, Study of Matter at Extreme Conditions 2011 (SMEC2011), an international conference hosted by the High Pressure Science Society of North America (HiPSSA); held on the *Liberty of the Seas*; March 2011.
2. “Predicting the Geometries and Electronic Structures of Compressed Solids”, 3rd International Symposium on Structure–Property Relationships in Solid States Materials, Stuttgart, Germany; July 2010.

1. “A Molecular Perspective on Lithium–Ammonia Solutions”, Cecam Workshop: Energy Landscape of Solids: from (hypothetical) topologies to material properties, Lausanne, Switzerland; July 2008.

Seminars

March 2020 - March 2022 virtual format; else in-person unless otherwise stated.

82. “Theoretical Design of Light-Element Superconductors and Other (Quantum) Materials”, Chicago/DOE Alliance Center (CDAC) Virtual Seminar Series; October 2023.
81. “Theoretical Design of Light-Element Superconductors and Other (Quantum) Materials”, Physics Colloquium, Rutgers-Newark; October 2023.
80. “Theoretical Design of Light-Element Superconductors and Other (Quantum) Materials”, Max Planck Institute for Solid State Research; August 2023.
79. “Theoretical Design of Light-Element Superconductors”, Dept MatSci & Eng, Carnegie Mellon University; April 2023.
78. “Theoretical Design of Light-Element Superconductors”, Dept MatSci & Eng, Johns Hopkins; Jan 2023.
77. “Theoretical Design of Light-Element Superconductors”, MatSci Research Lecture, Caltech; Jan 2023.
76. “Theoretical Design of Light-Element Superconductors”, Dept MatSci & Eng, University of Florida; Nov 2022.
75. “Theoretical Design of Light-Element Superconductors”, Dept Chem, University of Houston; Oct 2022.
74. “Theoretical Design of Light-Element Superconductors”, Dept Chem, Rice University; Oct 2022.
73. “Extreme Chemistry and New States of Matter at Extreme Pressures”, Dept Chem, SUNY Binghamton; Sept 2022.
72. “Extreme Chemistry and New States of Matter at Extreme Pressures”, Dept Chem, Canisius College, Buffalo; Sept 2022.
71. “Theoretical Design of Light Element Superconductors”, Monthly Meeting on Room-T Superconductivity, Asia Pacific Center for Theoretical Physics, Korea; July 2022 (virtual participation).
70. “Theoretical Predictions of Superconducting and Superhard Materials”, 75th Anniversary, Dept of Physics, Jilin University, China; March 2022.
69. “Extreme Chemistry and New States of Matter at Extreme Pressures”, Physics & Astronomy, California State University, CalPolyPomona; March 2022.
68. “Extreme Chemistry and New States of Matter at Extreme Pressures”, Dept Chem, St. Bonaventure; March 2022.
67. “Extreme Chemistry and New States of Matter at Extreme Pressures”, Dept Chem, California State University, San Bernardino; Feb 2022.
66. “Theoretical Predictions of Superconducting and Superhard Materials”, Condensed Matter Seminar, Case Western University; Oct 2021.
65. “Theoretical Prediction of Superconducting and Superhard Materials”, Namur Institute of Structured Matter Colloquium, Belgium; May 2021.
64. “Towards Room Temperature Superconductivity in Hydride-Based Materials Under Pressure?”, Condensed Matter Seminar, University California San Diego; April 2021.
63. “Towards Room Temperature Superconductivity in Hydride-Based Materials Under Pressure?”, Condensed Matter Seminar, University of Virginia; April 2021.
62. “Theoretical Predictions of Superconducting, Superhard and Catalytic Materials”, Dept Chem, University of Alabama; April 2021.

61. “Theoretical Predictions of Superconducting and Superhard Materials”, Materials Theory Group Journal Club, Oak Ridge National Laboratory; April 2021.
60. “Theoretical Predictions of Superconducting and Superhard Materials”, NSF Center for Mechanical Control of Chemistry Mechanochemistry Discussions; Feb 2021.
59. “Theoretical Predictions of Superconducting and Superhard Materials”, Fermilab Colloquium; Oct 2020.
58. “Towards Room Temperature Superconductivity in Hydride Based Materials Under Pressure?”, Theoretical Chemistry Seminar, University of Cambridge, UK; Oct 2020.
57. “Theoretical Predictions of Superconducting and Superhard Materials”, Theory and Simulation of Electronic and Optical Processes in Molecules and Materials Weekly Seminar; Oct 2020.
56. “Towards Room Temperature Superconductivity in Hydride Based Materials Under Pressure?”, MEMS/MatSci Seminar, Duke; Oct 2020.
55. “Theoretical Predictions of Superconducting and Superhard Materials”, Chicago/DOE Alliance Center (CDAC); May 2020.
54. “Theoretical Predictions of Superconducting and Superhard Materials”, HEDPt Workshop, Laboratory for Laser Energetics, University of Rochester; Feb 2020.
53. “Computational Discovery of New Materials Under Pressure”, MatSci and Engineering, Cornell; Sept 2019.
52. “Computational Discovery of New Materials Under Pressure”, MEMS/MatSci Seminar, Duke; Jan 2019.
51. “Chemistry Under Pressure”, Dept Chem, University of Richmond; Nov 2018.
50. “Chemistry Under Pressure”, Physical/Inorganic Chem, University of Wisconsin-Madison; March 2017.
49. “Predicting Materials Under Pressure”, Physics & Astronomy, University of Rochester; Feb 2017.
48. “Chemistry Under Pressure”, Physical Chem, Indiana University Bloomington; Feb 2017.
47. “Chemistry Under Pressure”, Dept Chem, Queens University, Kingston, ON, Canada; March 2016.
46. “The Structures of Methylaluminoxane (MAO) in Homogeneous and Heterogeneous Phases”, Collaborative Research Center on Understanding Metal Oxide / Water Systems at the Molecular Scale Seminar, Technische Universität Berlin, Germany; May 2015.
45. “Chemistry Under Pressure”, Prof. Nicola Spaldin’s Group Seminar, ETH Zürich; March 2015.
44. “Chemistry Under Pressure”, Theory Department, Max Planck Institute of Microstructure Physics, Halle, Germany; March 2015.
43. “Chemistry Under Pressure”, Competence Center for Computational Chemistry “C4” Seminar, ETH Zürich; March 2015.
42. “Chemistry Under Pressure”, Dept Chem; University of Calgary; Canada; Jan 2015.
41. “Structure Prediction from First Principles Calculations”, Dept Chem; Texas Women’s University; March 2014.
40. “Building a Chemical Intuition Under Pressure: Prediction of Alkali Metal Polyhydrides”, Condensed Matter Seminar, University of Toronto; Canada; Oct 2013.
39. “Building a Chemical Intuition Under Pressure: Prediction of Alkali Metal Polyhydrides and Subhydrides”, Dept Chem; SUNY Geneseo; Oct 2013.
38. “Building a Chemical Intuition Under Pressure: Prediction of Alkali Metal Polyhydrides and Subhydrides”, Inorganic/Physical Seminar; University of Rochester; Sept 2013.
37. “Building a Chemical Intuition Under Pressure: Prediction of Alkali Metal Polyhydrides and Subhydrides”, High Pressure Seminar, Max Planck Institut für Chemie, Mainz; Germany; June 2013.
36. “Structure Prediction from First Principles”, Phys/MatSci Colloquium, SUNY Binghamton; April 2013.

35. “Building a Chemical Intuition Under Pressure: Prediction of Alkali Metal Polyhydrides and Subhydrides”, Dept Chem, University of Delaware; March 2013.
34. “Building a Chemical Intuition Under Pressure: Prediction of Alkali Metal Polyhydrides and Subhydrides”, Condensed Matter Seminar; University of Utah; Feb 2013.
33. “Insulating Na and Metallic H_2: Developing a Chemical Intuition Under Pressure”, Chem/MatSci, Rochester Institute of Technology; Jan 2013.
32. “Building a Chemical Intuition Under Pressure: Prediction of Alkali Metal Polyhydrides and Subhydrides”, Condensed Matter Seminar; Rutgers University; Jan 2013.
31. “Insulating Na and Metallic H_2: Developing a Chemical Intuition Under Pressure”, Penn-York Section of ACS; Nov 2012.
30. “Building a Chemical Intuition Under Pressure - Alkali Metals, their Polyhydrides and Subhydrides”, Dept Chem; University of Warsaw; Poland; July 2012.
29. “Building a Chemical Intuition Under Pressure - Alkali Metals, their Polyhydrides and Subhydrides”, Dept Chem; University of Western Ontario; Canada; March 2012.
28. “Building a Chemical Intuition Under Pressure - Alkali Metals, their Polyhydrides and Subhydrides”, Dept Chem; University of Guelph; Canada; Feb 2012.
27. “Insulating Na and Metallic Hydrogen — Developing a Chemical Intuition Under Pressure”, Dept Chem; Oakland University; Feb 2012.
26. “Research in the Zurek Group”, Integrated Nanostructured Systems, SUNY Buffalo; Jan 2012.
25. “Alkali Metal Polyhydrides/Subhydrides Under Pressure”, Quantum Simulation Group, LLNL; Dec 2011.
24. “Novel Hydrogen Rich Phases Under Pressure”, Nebraska Center for Materials and Nanoscience, University of Nebraska–Lincoln; Nov 2011.
23. “Insulating Na and Metallic Hydrogen — Developing a Chemical Intuition Under Pressure”, Dept Chem; Daemen College, Buffalo; Nov 2011.
22. “Insulating Na and Metallic Hydrogen — Developing a Chemical Intuition Under Pressure”, Dept Chem; Penn State Erie the Behrend College; Oct 2011.
21. “Insulating Na and Metallic Hydrogen — Developing a Chemical Intuition Under Pressure”, Dept Chem; Canisius College, Buffalo; Sept 2011.
20. “From Alkali Metals to Superalkalis”, Vrije Universiteit of Amsterdam, the Netherlands; July 2011.
19. “Predicting the Geometries and Electronic Structures of Solids with Genetic Algorithms”, Dept Chem; Middle Tennessee State University; Nov 2010.
18. “Predicting the Geometries and Electronic Structures of Compressed Solids”, Dept Physics; Brock University, St. Catherine’s, Canada; Nov 2010.
17. “Two Tales about the Third Element”, Integrated Nanostructured Systems Meeting, SUNY Buffalo; April 2010.
16. “Two Tales about the Third Element”, Dept Chem; SUNY Brockport; April 2010.
15. “Two Tales about the Third Element”, Dept Chem; Michigan Tech University; March 2010.
14. “Two Tales about the Third Element”, Dept Chem; John Carroll University; Feb 2010.
13. “A Little Bit of Lithium Does a Lot for Hydrogen”, Physics Colloquium; SUNY Buffalo; Feb 2010.
12. “Two Tales about the Third Element”, Dept Chem; Siena College; Nov 2009.
11. “Theoretical Studies of Complex Chemical Systems”, Dept Chem; Syracuse University; Jan 2009.
10. “Theoretical Studies of Complex Chemical Systems”, Dept Chem; SUNY Buffalo; Jan 2009.

9. “A Molecular Perspective on Lithium–Ammonia Solutions”, Max Planck Institute for Solid State Research, Stuttgart; July 2008.
8. “DFT Studies of the ^{13}C NMR Chemical Shifts of Single-Walled Carbon Nanotubes (SWNTs)”, CNRS, Lyon, France; Feb 2007.
7. “DFT Studies of the ^{13}C NMR Chemical Shifts of SWNTs, Magic Metal-$(C_{60})_2$ Clusters and *N*MTO Wannier-like Functions for Solids”, Brookhaven National Lab and Stony Brook University; Oct 2006.
6. “Wannier–like Functions for Metals and Intermetallic Compounds”, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany; Sept 2006.
5. “DFT Studies of the ^{13}C NMR Chemical Shifts of SWNTs and *N*MTO Wannier-like Functions for Solids”, Vrije University of Amsterdam; Netherlands; Aug 2006.
4. “Computational Studies of Magic Metal-$(C_{60})_2$ Clusters”, *Arbeitsbeschprechung*, Max Planck Institute for Solid State Research; Stuttgart; May 2005.
3. “Computational Studies of MAO and SWNTs”, Imperial College of London, UK; March 2005.
2. “Modeling MAO (Methylaluminoxane)”, Basell Polyolefins, Ludwigshafen, Germany; March 2003.
1. “Modeling MAO (Methylaluminoxane)”, Jagiellonian University, Kraków, Poland; Feb 2003.

Research Group

Visiting Scholars
Prof. Jose Manuel Recio (2022); University of Oviedo; Spain
Prof. Miao Zhang (2019-2020); Beihua University; Jilin, China
Prof. Yan Yan (2019-2020); Changchun University; Jilin, China
Prof. Mariusz Kozik (2013-2014); Canisius College; Buffalo
Prof. Bahadir Altintas (2011-2012); Abant Izzet Baysal University; Turkey
PhD. Student Antonio Rivera Brown (2011); University Puerto Rico Mayaguez

Postdoctoral Associates - Present
Francesco Belli (2023-present)
Samad Hajinazar (2023-present)
Dongbao Luo (2022-present)
Busheng Wang (2021-present)
Biswas Rijal (2021-present)
Josiah Roberts (2021-present)
Stefano Racioppi (2021-present)
Xiaoyu Wang (2023 - present)
Nisha Geng (2023-present)

Postdoctoral Associates - Former
Katie Hilleke (2019-2023); Assistant Scientist, Laboratory for Laser Energetics, Rochester
Pratik Kumar Das (2021-2022); INSPIRE Faculty Fellow, IIEST Shibpur, Kolkata
Niloofar Zarifi (2016-2018); Teaching / R&D in Canada
Nina Tyminska (2013-2015); Researcher in France
Xiaoguong Luo (2013-2014); Professor at Nankai University, China
James Hooper (2011-2013); Researcher Jagiellonian University, Kraków, Poland
Pio Baettig (2009-2011); R&D in Switzerland

Current Doctoral Students
Masashi Kimura (2021-present)
Trevor Higgins (2023-present)
Morgan Redington (2019-present)

PhD. Graduates, Year, Initial Position

- Nisha Geng, 2023; *First-Principles Calculations for Materials Design: From 1 atm to High Pressure*; Postdoc Zurek Group.
- Xiaoyu Wang, 2023; *Density Functional Theory Studies of High-Pressure Hydrides and Superhard Carbon Materials*; Postdoc Zurek Group.
- Tiange Bi, 2020; *Density Functional Theory Studies of Hydrogen Rich Materials, Methylammonium Lead Bromide Perovskite, and Silicon Dioxide Under Pressure*; Postdoc Geophysical Laboratory, Carnegie Institute, DC.
- Patrick Avery, 2019; *Open Source Software for the Prediction of Crystal Structures and the Analysis of their Properties*; R&D Engineer at *Kitware*.
- Daniel Miller, 2018; *Interactions at the Surface-Adsorbate Interface: An Outlook Through Computational Work*; Assistant Professor at Hofstra University.
- Zack Falls, 2017; *Elucidating Chemical Structures via DFT Investigations*; NLM University-based Biomedical Informatics Research Training Award from the NIH, Postdoctoral Fellow at the Department of Biomedical Informatics, Jacobs School of Medicine and Biomedical Sciences, UB, advisor: Prof. Ram Samudrala.
- Andrew Shamp, 2017; *Density Functional Theory (DFT) Studies of Hydrogen Rich Solids and Boron Carbide Under Extreme Conditions*; National Nuclear Security Administration Postdoctoral Fellowship, Washington, D.C.
- Tyson Terpstra, 2016; *Theoretical Investigations of Dense Hydrides and Complex Intermetallics*; Assistant Professor at D'Youville College.
- Scott Simpson, 2014; *Theoretical Investigations of Surface-Adsorbate Interfaces*; Assistant Professor at St. Bonaventure University.
- David Lonie, Ph.D. 2013; *Open Source Chemistry: Creating Tools for Automated Structure Prediction, Modeling, Visualization, and Analysis*; R&D Engineer at *Kitware*.

MSc. Graduates, Year, Initial Position

- Seong Won Jang, 2023; *Investigation of Superconductivity in Ternary Hydride Systems Under Pressure*; Dental School.
- Michelle Jabbour, 2017; *Computational Study of Surface-Adsorbate Interactions*; Lab Coordinator/Instructor at D'Youville College.
- Kyle Whitson, 2012; *Density Functional Theory Studies of Gold Clusters*; Praxair.

Undergraduates

Cooper Cohen (2022-2023), UB
Giacomo Scilla (2022-2023), UB
Nicholas Nasr, (2022), CSUSB
Zanaya Hussein (2022), UB
Katie Grove, (2018), CSUSB
Jose Uribe, (2017), CSUSB
Moises Romero, (2016), CSUSB
Shannon McDonnell, (2016) Penn State Erie, Behrend
Nathan Tierce, (2015), CSUSB
Andrew Lawrence, (2015), Penn State Erie, Behrend
Susanne Simkovitch, (2014), Penn State Erie, Behrend
Carlos Mora, (2014), CSUSB
Lara Hargrave, (2014), UB
Patrick Saitta, (2014), UB
Alex van Fleet (2013), UB
Jessica Rogers (2013), UB
Jiechen Chen, (2011-2012), UB, 'URGE to compute'
Amanda Wach, (2011-2012), UB, 'URGE to compute'
Daniel Poore (2012), UB
Sean Settlock (2012), UB
James Pander, (2011), Penn State Erie, Behrend, REU
Zack Falls, (2011), Canisius, REU

Student & Postdoc Awards

- Morgan Redington: Mattern–Tyler Teaching Award (2021), John Rys Scholarship (2022), Energy Efficiency and Renewable Energy (EERE) Energy Storage Summer Internship (2023)
- Nisha Geng: John Rys Scholarship (2021), APS DCMP Graduate Travel Award
- Xiaoyu Wang: John Rys Scholarship (2019), James T. Grey Jr. Summer Fellowship (2020), APS DCOMP Student Travel Award (2022)
- Tiange Bi: New York State APS Symposium 3rd Place Poster Award in the Graduate Category (2017), APS DCOMP Student Travel Award (2019), UB Chemistry Best PhD Dissertation Award Prize
- Zack Falls: 2017 "NLM University-based Biomedical Informatics Research Training" Award from the NIH
- Daniel Miller: Speyer Fellowship (Spring 2017)
- Patrick Avery: Google Summer of Code (Summer 2016), Phase-I Software Fellowship from the Molecular Sciences Software Institute (2017), UB Chemistry Best PhD Dissertation Award Finalist
- Patrick Saitta: *Science Undergraduate Laboratory Internship* from the DOE (2013)
- Jiechen Chen: *Gehmen Scholarship*, for her ability in math and interest in math education (2013)
- James Hooper: *HOMING PLUS* fellowship from the Foundation for Polish Science (2013-2015)
- David Lonie: Google Summer of Code (Summer 2011), Speyer Fellowship (Spring 2012)
- Andrew Shamp: 2012 Computational Chemistry and Materials Science Summer Institute at LLNL, Joint APS-SCCM/AIRAPT Conference Student Travel Scholarship (2013), First Prize in Student Poster Session: High Pressure Chemistry at the 96th Canadian Chemistry Conference and exhibition, 2017 National Nuclear Security (Post)Graduate Fellowship, UB Chemistry Best PhD Dissertation Award Finalist
- Scott Simpson: Mattern–Tyler Teaching Award (2012), Graduate Student Excellence in Teaching Award (2013), College of Arts and Sciences Dissertation Fellowship (2014)
- Tyson Terpstra: Student Poster Award GRC on High Pressure (2014), Mattern–Tyler Teaching Award (2015)

Student Advisement

Dissertation Committee Member (major professor in parentheses)
Farnoush Nourigheimasi (Autschbach), Morgan Redington (Zurek), Herbert Ludowieg (Autschbach), Mahsa Jabbar (Akimov), Nisha Geng (Zurek), Xiaoyu Wang (Zurek), Adam Phillips (Autschbach), Michelle Gabour (Zurek), Patrick Avery (Zurek), Tiange Bi (Zurek), Sabry Gad Al Hak Moustafa (Kofke), Alex Marchenko (Autschbach), Thomas Duigan (Autschbach), Dan Miller (Zurek), Zackary Falls (Zurek), Tyson Terpstra (Zurek), Robert Martin (Autschbach), Doreen Prendergast (Watson), Sanghamitra Sengupta (Velarde), Jordan Cox (Benedict), Heather Rudolph (Wood), Ben Pritchard (Autschbach), Lucia Nitsch (Autschbach), Mark Rudolph (Autschbach), Kiplangat Sutter (Autschbach), Barry Moore (Autschbach), Brian Schultz (Banerjee), Peter Marley (Banerjee), Katie Farley (Banerjee), Robert Dennis (Banerjee), Kate Pelcher (Banerjee), Thomas O'Loughlin (Banerjee), Jesse Sokolow (Coppens), Timothy Halter (Nancollas), David Lonie (Zurek), Kyle Whitson (Zurek), Scott Simpson (Zurek), Andrew Shamp (Zurek)

External Member of PhD. Committee (major professor in parentheses)
Surender Singh, Department of Chemistry, Indian Institute of Technology, Kanpur (DLVK. Prasad); Simone di Cataldo, Faculty of Physics, TU Graz, Austria (L. Boeri); Yaoting Zhang, Department of Chemistry, Queen's University, Canada (N. Mosey); Sabri Elatresh, Department of Physics, Dalhousie University, Canada (S. Bonev); Sarina Bellows, Chemistry Department, University of Rochester (P. Holland); Silvia Bahmann, Faculty of Chemistry and Physics, TU Bergakademie Freiberg, Germany (J. Kortus)

Mentoring

- Mentor in the URGE (Undergraduate Research Group Experiences) to Compute Program (2011-2012), funded by the NSF's CSUMS program in collaboration with the UB and Buffalo State Mathematics Department, UB Physics, the CCR and HWI. I supervised two female undergraduate students (Jiechen Chen: double major in chemistry and applied mathematics, Amanda Wach: double major in biomedical engineering and mathematics). The students conducted a year-long research project supervised by myself, presented their work at the Spring ACS meeting in New Orleans, and a paper on their work has been published *Analytical Chemistry*.

- External partner for California State University San Bernardino (CSUSB) NSF-CREST grant. CSUSB is a primarily undergraduate minority serving institution. Each year 2-3 CSUSB students receive funds to participate in an REU-like experience at UB. The CSUSB students I have mentored are listed above in the "Past Undergraduates" section. Furthermore, two of my PhD students spent 1 quarter teaching at CSUSB, and was closely supervised by a CSUSB faculty mentor.

Teaching

Courses Taught

- Chemistry 102, General Chemistry II (Spring 2021).
- Chemistry 290, Undergraduate Research Supervision (Fall 2011).
- Chemistry 319, Physical Chemistry I for Undergraduates (Fall 2016, 2018).
- Chemistry 330, Physical Chemistry Lab: Computational Chemistry (Spring 2012-2016, 2018-2023).
- Chemistry 334, Physical Chemistry for Engineers (Fall 2010-2013, 2023).
- Chemistry 498, Senior Research Supervision (Spring/Fall 2012-2014).
- Chemistry 458/506, Physical Chemistry II for Graduate Students (Spring 2011).
- Chemistry 457/505, Physical Chemistry I for Graduate Students (Fall 2009-2013, 2021).
- Chemistry 512, Modern Materials: Theory, Applications, and Advanced Characterization Techniques (Fall 2012).
- Chemistry 571, Advanced Laboratory Techniques (Spring 2010, Fall 2014).
- Chemistry 720, Graduate Research Supervision (Academic Year 2010-2023).

Course Development

- *Chemistry 330:* I developed a completely new Undergraduate Computational Chemistry Laboratory course. The lab is held in one of the science and technology classrooms at UB and the computational experiments are performed on the supercomputing cluster housed and maintained by UB's Center for Computational Research (CCR). Computations are carried out using the *WebMO* interface to Gaussian, and the molecular editor Avogadro is employed to build molecules and perform force–field optimizations. I developed a number of new computational experiments performed in the lab that have been published in the *Journal of Chemical Education* [43, 44, 49, 50, 119, 167], and my student wrote an extension to Avogadro to build and visualize the SWNTs for one of these experiments [43].
- *Chemistry 512:* This was a special topics course team-taught by Dr. Jason Benedict and myself. I focussed on introducing students to band structure theory using a chemist's perspective. The course was inspired by Roald Hoffmann's book "Solids and Surfaces: A Chemist's View of Bonding in Extended Structures", Jeremy Burdett's book "Chemical Bonding in Solids" and Whangbo's review article "Conceptual Aspects of Structure-Property Correlations and Electronic Instabilities, with Applications to Low-Dimensional Transition-Metal Oxides". Topics included: Hückel (or tight–binding) calculations, band structures and densities of states, reciprocal space, crystal orbital overlap populations, Fermi surfaces and Brillouin zones, Peierls distortions and Fermi surface nesting, electron-phonon coupling, the free electron gas model.
- *Chemistry 457/505:* This course was updated and a new section on modern electronic structure methods in chemistry was been added. Exercises using the WebMO interface to Gaussian are employed to introduce students to computational software.
- *Chemistry 334:* This course was updated and a section introducing students to computational methods in chemistry was added. Exercises using the WebMO interface to Gaussian were introduced. I helped my collaborator, Dr. Autschbach, develop exercises on band structure and my student interfaced YAeHMOP with Avogadro to be used for these exercises [97].

Service

Departmental

- Personnel Committee (2022-present)
- Graduate Curriculum, Advisement and Petitions Committee (2018-2023)
- Chair Colloquium Committee (2022 - present)
- Colloquium Committee (2012 - present)

- Undergraduate Committee (2021 - 2023)
- Executive Committee (2018-2020)
- ATOMS Convenor (2018-2020)
- Space Committee (2018-2019)
- Awards Committee Chair (2016-2019)
- Awards Committee (2014-2019, 2023-present)
- Graduate Admissions Committee (2010-2018)
- Recruiting Committee (2009-2016)
- Website Redesign Committee (2014)
- Safety Committee (2010)
- Physical Chemistry Faculty Search Committee (2014)
- Analytical Chemistry Faculty Search Committee (2013)
- Materials Science and Engineering / Chemistry Faculty Search Committee (2012)
- Computational Physics Faculty Search Committee (2023-present)
- Materials Chemistry Faculty Search Committee (2023-present)

University

- Member of UB Vice President University Libraries Search Committee (2017)
- Appeared in a video promoting UB's Center for Materials Informatics (2014)
- Judge for PhD Poster Competition in Chemical and Biological Engineering (2014)
- Chemical and Biological Engineering Faculty Search Committee, External Member (2014)
- Mentor in URGE to Compute Program (2012-2013)
- Faculty Advisory Board, Polish Studies Program (2010-2012)
- Hosted Chemical and Biological Engineering Faculty Candidates (2012, 2013)

Professional

- Working group leader for the *Multi-Petawatt Physics Prioritization Workshop* (2021-2022), `https://arxiv.org/pdf/2211.13187.pdf`.
- Reviewer of the report *Fundamental Research in High Energy Density Science*, from the Board on Physics and Astronomy (BPA) of the National Academies of Sciences, Engineering and Medicine (2022), `https://nap.nationalacademies.org/catalog/26728/fundamental-research-in-high-energy-density-science`.
- Reviewer of grant proposals from the National Science Foundation (Divisions of Chemistry & Materials Research & Earth Sciences), the ACS Petroleum Research Fund, the US Department of Energy (BES), the National Nuclear Security Agency.
- Reviewer of grants from international funding agencies, e.g. Austrian Research Fund (2019), Partnerships for Advanced Computing in Europe (2018), National Science Center, Poland (2016), NSERC, Canada (2015), CRDF Global (2014), Deutsche Forschungsgemeinschaf (2014), Hungarian Scientific Research Fund (2014), Austrian Academy of Sciences (2013), Indian Institute of Technology (2013).
- Editorial Board Member *Physical Review Materials*, Jan 2021-present.
- Member of the Editorial Advisory Board of *Organometallics*, 2020-2022.
- Elected as a "Vice Chair" for the *American Physical Society Division of Computational Physics* (APS-DCOMP), March 2022-2026.
- Elected as a "Member at Large" for the *American Physical Society Division of Computational Physics* (APS-DCOMP), March 2019-2022.
- Member of the Editorial Advisory Board of *Crystals*, MDPI Open Access Journals, April 2019-present.
- Member of the Editorial Advisory Board of the *International Journal of Quantum Chemistry*, Wiley, Feb 2018-present.
- Section Editor for "Electronic Structure" for *Journal of Physics: Condensed Matter*, 2017-2021.
- Member of the Editorial Advisory Board of *Journal of Physics: Condensed Matter*, Institute of Physics, 2016-2021.
- Member of Editorial Advisory Panel for *Scientific Reports*, Nature Publishing Group, Nov 2014 - April 2019.
- Member of the Advisory Board for the *International Conference on Chemical Bonding*, 2015.
- Review about 40-50 manuscripts per year in top-rated chemistry, physics and materials science journals.
- Refereed book proposal *Bonding Models in Code: An Entry into the Theoretical Chemistry of Inorganic Molecules and Materials*, Taylor and Francis/CRC Press (2015).

- Refereed *Cooksy Physical Chemistry* published by Pearson Higher Education (2011).
- Regular member of the American Chemical Society, and the American Physical Society.
- *Matter at Extreme Conditions* Focus Session, 2022 March APS Meeting, co-organized with John Borg, Peter Celliers, Ivan Oleynik, Nenad, Velisavlejevic.
- *Matter in Extreme Environments* Focus Session, 2021 March APS Meeting, co-organized with Gilbert Collins, Shanti Deemyad, Andreas Hermann, Antonio Moreira Dos Santos, Koichiro Umemoto.
- *Matter in Extreme Environments* Focus Session, 2019 March APS Meeting, co-organized with Paul Loubeyre, Yanming Ma, Jon Eggert, Maosheng Miao and Bianca Haberl.
- *Materials in Extreme Environments*, Fall 2018 ACS Meeting, co-organized with Anastassia Alexandrova.
- *Symposium in Honor of Roald Hoffmann*, Fall 2017 ACS Meeting, co-organized with Wojciech Grochala.
- *Structure and Electronic Structures of Ultra Light Materials*, and *Computational Materials Structure and Property Predictions – Methods and Applications for High Pressure and Low-Dimensional Systems*, Studies of Matter at Extreme Conditions, 04/2017, co-organized with Shanti Deemyad and Richard Hennig.
- *High Pressure Chemistry*, Canadian Society for Chemistry 2013, co-organized with Yansun Yao and John Tse.
- Referee of hiring/promotion/tenure cases in the USA, UK, Europe and Isreal

Public Service and Outreach

- 2020-2023: Interviewed by the *New York Times*, *Chemistry World*, *Nature*, *QuantaMagazine*, *Scientific American*, *New Scientist*, *Science*, *Chemistry & Industry*, *UB*, *Popular Science* and more regarding breakthroughs in superconductivity research & high-pressure science.
- 2019: Interviewed by *Popular Mechanics*, *Chemistry World*, *Sztuczna Inteligencja* regarding discovery of superhard materials.
- 2019: Interviewed by Robert Henderson for a feature article on superconductivity that was published in the October 2019 issue of *Scientific American*.
- 2018/19: Interviewed by *Science News*, *Chemistry World*, the Canadian Broadcasting Corporation's *Quirks & Quarks*, National Public Radio's *Science Friday*, and *C&EN News* about the high temperature superconductivity measured in a hydride of lanthanum under pressure.
- 2017/18: Interviewed by *Scientific American*, *Chemistry World*, *Inside Science* and *C&EN News* about the reactivity of helium under pressure.
- Gave a public lecture on improvisation in science at Buffalo's "16th Science and Art Cabaret".
- Appeared in a Youtube video regarding UB's research in materials informatics.
- Speaker at high-school/undergraduate/graduate summer schools (e.g. Eric Pitman Summer Workshop in Computational Science, LLNL Computational Chemistry and Materials Science Summer Institute, Center for Matter at Atomic Pressures Undergraduate Summer School).
- Speaker promoting women in science (e.g. WoPhys Conference for Undergraduate Women in Physical Sciences, Texas Women's University).