

CURRICULUM VITAE

JOSEPH W. BENNETT

Assistant Professor
Department of Chemistry & Biochemistry
University of Maryland, Baltimore County
1000 Hilltop Circle
Baltimore, MD 21250

EDUCATION

Ph.D.	2009	University of Pennsylvania (Philadelphia, PA), Chemistry
B.S.	2003	Drexel University (Philadelphia, PA), Chemistry

Experience in Higher Education

July 2024 – present	University of Maryland College Park , College Park, MD Adjunct Professor of Materials Science & Engineering
August 2021 – present	University of Maryland Baltimore County , Baltimore, MD Assistant Professor of Chemistry
July 2019 – August 2021	University of Maryland Baltimore County , Baltimore, MD, College of Natural and Mathematical Science Pre-Faculty Fellowship
April 2016 – June 2019	University of Iowa , Iowa City, IA Research Specialist in the Department of Chemistry
April 2015 – April 2016	Rutgers University , New Brunswick, NJ Staff Scientist in the Department of Physics and Astronomy
Jan. 2010- October 2012	Rutgers University , New Brunswick, NJ Postdoctoral research associate in the Department of Physics and Astronomy
June- December 2009	University of Pennsylvania , Philadelphia, PA Post-doctoral training in the Department of Chemistry

Experience in Other Than Higher Education

July 2014 - present	Aqua Vectors, Inc. , Northport, NY Scientific consultant and collaborator
Oct. 2012 – July 2014	Eos Energy Storage , Edison, NJ Research Manager

Honors and Awards

2021	UMBC START grant FY21
2019-2021	UMBC College of Natural and Mathematical Science Pre-Faculty

	Fellowship in the Department of Chemistry and Biochemistry
2009	John G. Miller Award for Most Outstanding Doctoral Thesis in Chemistry, University of Pennsylvania
2004	GAANN Fellowship, University of Pennsylvania
2003	Robert O. Hutchins BIOMOL Prize for Research, Drexel University
2003	American Institute of Chemists Award, Drexel University
2003	Chemists Club of Philadelphia Scholarship, Drexel University
2002	Bruce and Cynthia Maryanoff Research Prize, Drexel University

External Recognition

- July 2025 EurekaAlert! “New computational method predicts novel 2D materials for electronics” (AAAS)
- February 2024 Cover article, February 2024 issue of *Surface Science*
- January 2023 Featured in *J. Phys. Chem. C*. “Early Career and Emerging Researchers Vol. 2” issue (ACS)
- December 2022 Cover article, December 2022 issue of *Surface Science*
- August 2022 Featured in Physics Synopsis “Semiconductors in the Spotlight” (APS)
- April 2022 Featured in *Inorg. Chem.* “Out in Inorganic Chemistry: A Celebration of LGBTQIAPN+ Inorganic Chemists” issue (ACS)
- January 2022 Featured in *J. Mater. Res.* “Early Career Scholars in Materials Science” issue (MRS)

Research Support

2024-2029	“Designing Multiferroic Composites from Layered Ferroelectric Chalcogenides and van der Waals Ferromagnets” <u>source</u> : DTRA, <u>role</u> : co-PI, <u>amount awarded</u> \$2,500,000 (UMBC: \$744,000)
2020 – 2021	Recipient of FY21 START grant, <u>source</u> : UMBC, <u>role</u> : PI, <u>amount awarded</u> : \$24,000
2020 – 2021	Recipient of Funds to Continue Work on Environmental Chemistry, <u>source</u> : Middendorf Foundation, <u>role</u> : PI, <u>amount awarded</u> : \$10,000
2025	“CAREER: Database-Enabled Discovery and Design of Ferroics to Broaden Participation in Materials Theory and Computing” <u>source</u> : NSF, <u>role</u> : PI, <u>amount requested</u> : \$603,000 (under review)
2025	“Collaborative Research: DMREF: High-throughput Design and Discovery of Emerging van der Waals Multiferroics for Atomically Thin Spintronics” <u>source</u> : NSF, <u>role</u> : co-PI, <u>amount requested</u> : \$382,000 (under review)
2025	“REU Site: A Summer Research and Training Program in Art Conservation Science Exploring the Interface between Science and Art (SCIART),” <u>source</u> : NSF <u>role</u> : senior personnel, <u>amount requested</u> : \$541,000 (under review)

review)

- 2024 “NSF Engineering Research Center for AI-driven Design of Responsive Engineered Advanced Materials (AI-DREAM),” *source*: NSF, *role*: co-PI (declined)
- 2024 “REU Site: A Summer Research and Training Program in Art Conservation Science Exploring the Interface between Science and Art (SCIART),” *source*: NSF, *role*: senior personnel (declined)
- 2024 “CAREER: Combining Databases, Discoveries, and Design to Broaden Participation in Materials Theory and Computing” *source*: NSF, *role*: PI, *amount requested*: \$786,569 (declined)
- 2024 “GOALI: Reliable Adsorption of Contaminants through Surface Interaction: Deploying Amorphous Hydroxides to Reliably Treat Contaminated Water” *source*: NSF, *role*: PI, *amount requested*: \$504,970 (declined)

Computational Support

- 2025 “A First-Principles Informed Machine Learning Model for 1D Multiferroic Materials for Electronics and Medicine” *source*: DOE, *role*: PI, CFN GUP 318985 *awarded* 378,000 computing SU
- 2025 “Chiral Adsorbates Used to Tune Light-Matter Interactions of Organic-Inorganic Multiferroics” *source*: DOE, *role*: PI, CFN GUP 317953 *awarded* 304,000 computing SU
- 2024 “1D Multiferroic Materials for Electronics and Medicine” *source*: DOE, *role*: PI, CFN GUP 315016/317084 *awarded* 590,000 computing SU
- 2024 “Novel 2D Chalcogenide Composites for Microsensors” *source*: DOE, *role*: PI, CFN GUP 315013 *awarded* 240,000 computing SU
- 2019 –2023 “Atomistic Insights into Safer Water and Cleaner Energy from Density Functional Theory”, *source*: NSF-XSEDE, *role*: PI, *total awarded*: 1,200,000+ computing SU
- 2022 “DFT Methods as a Noninvasive Probe for Art Conservation Science in the Baltimore SCIART Summer Program”, *source*: NSF-XSEDE, *role*: PI, *awarded*: 50,000 computing SU

Ph.D. Students

- Mona Layegh, degree awarded 7/2025, *Role*: PhD advisor/committee Chair
- Anthony Casale, degree expected in 2026, *Role*: PhD advisor/committee Chair
- Peng Yan, degree expected in 2027, *Role*: PhD advisor/committee Chair
- Yussuf Fasasi, degree expected in 2030, *Role*: PhD advisor/committee Chair

Undergraduate Students

- Stephen Shaner, UMBC undergraduate research (April 2025-present), Role: research mentor
- Mei Liu, UMBC undergraduate research (August 2023-May 2024), degree awarded in 2024, Role: research mentor
- Caitlin Doherty, UMBC undergraduate research (June 2023-May 2024), degree awarded in 2024, Role: research mentor
- Rachel Rehling, UMBC undergraduate research (June 2023-December 2023), degree awarded in 2023, Role: research mentor
- Rayal Smith, UMBC undergraduate research & LSAMP scholar (June 2023-May 2024), degree awarded in 2024, Role: research mentor
- Joshua Birenzige, UMBC undergraduate research (December 2022-May 2023), degree awarded in 2023, Role: research mentor
- Aria Tauraso, Merck Undergraduate Fellow & UMBC undergraduate research (June 2022-present), Role: research mentor
- Amalthea Trobare, UMBC undergraduate research (June 2022- May 2024), degree awarded in 2024, Role: research mentor
- Eunice Costanzo, Merck Undergraduate Fellow & UMBC undergraduate research (May 2022-May 2023), degree awarded in 2024, Role: research mentor
- Lila Marino, Merck Undergraduate Fellow & UMBC undergraduate research (May 2022-May 2023), degree awarded in 2023, Role: research mentor
- Jasper Tucker, UMBC undergraduate research (August 2021-June 2022), degree awarded in 2022, Role: research mentor
- Aaliyah Khan, UMBC undergraduate research & LSAMP Scholar (August 2020-June 2022), degree awarded in 2022, Role: research mentor
- Autumn Cook, UMBC undergraduate research (August 2020-June 2021), degree awarded in 2021, Role: research mentor
- Ryan Grimes, UMBC undergraduate research (March 2020-present), degree awarded in 2021, Role: research mentor
- Joshua Leginze, UMBC undergraduate research (March 2020-July 2021), degree awarded in 2021, Role: research mentor
- Robert Zochowski, UMBC undergraduate research (March 2020-August 2020), graduated August 2020, Role: research mentor

High School Students

- Iffat Chowdhury, Al-Huda High School 2025, Role: research mentor
- Skye Eliot, Blair Montgomery High School 2022-2024, Role: research mentor
- Stanley Ou, Blair Montgomery High School 2021, Role: research mentor

Student Awards

- Aria Tauraso, Outstanding Graduating Senior Award, UMBC Chemistry & Biochemistry, May 2025

- Stephen Shaner, MERCK fellow “Data Sciences in the Life Sciences”, UMBC CNMS, April 2025
- Aria Tauraso, ACS Physical Chemist Award, UMBC Chemistry & Biochemistry, April 2024
- Anthony Casale, Army Education Outreach Program (\$74,800/yr), Sept 2023-Feb 2025
- Aria Tauraso, CNMS Scholars Program for 2023-2024, August 2023
- Aria Tauraso, MERCK fellow “Data Sciences in the Life Sciences”, UMBC CNMS, May 2023
- Amalthea Trobare, ACS Physical Chemist Award, UMBC Chemistry & Biochemistry, April 2023
- Jasper Tucker, Vitullo Research Award, UMBC Chemistry & Biochemistry, May 2022
- Aaliyah Khan, ACS Chesapeake Award, UMBC Chemistry & Biochemistry, May 2022
- Lila Marino, MERCK fellow “Data Sciences in the Life Sciences”, UMBC CNMS, May 2022
- Eunice Costanzo, MERCK fellow “Data Sciences in the Life Sciences”, UMBC CNMS, May 2022
- Ryan Grimes, Vitullo Research Award, UMBC Chemistry & Biochemistry, May 2021
- Aaliyah Khan, Satterfeld Award, UMBC Chemistry & Biochemistry, May 2021
- Autumn Cook, Mittino Service Award, UMBC Chemistry & Biochemistry, May 2021

PUBLICATIONS

Peer-refereed Works

Articles

1. A. Casale and J. W. Bennett, “Insulating A_2VX_3 Oxides and Sulfides as Ferromagnetic Wires”, (*under review*)
2. P. Yan, A. Casale, and J. W. Bennett, “Modeling 2D van der Waals Materials with Homonuclear Bonds of Main Group Cations”, (*in press, ACS Au Organic & Inorganic*) 11/2025
3. M. Layegh and J. W. Bennett, “Compositional Design Rules for Tuning Functionalities in $CuInP_2X_6$ ($X=S, Se$) van der Waals Semiconductor Ferroelectrics”, *Dalton Trans.*, 2025, (54), 14384-14395
4. M. Lopez, P. Yan, P. Zavalij, A. Javadi, I. da Silva, Z. Wang, S. Ren, J. W. Bennett, E. E. Rodriguez, “Evidence of Ferrimagnetism in Fe_3GeTe_2 via Neutron Diffraction Studies”, *J. Mater. Chem. C.*, 2025, (13), 15354-15361
5. P. Yan, M. Layegh, R. Stadel, J. Birenzvice, P. Y. Zavalij, E. E. Rodriguez, J. W. Bennett, “Data-Enabled Discovery of 2D van der Waals Layered Phosphochalcogenides”, *Chem. Mater.*, 2025, (37), 5086-5098
6. M. Layegh and J. W. Bennett, “Open-Source DFT Calculations of Electronic Structure to Understand Bonding in Solids”, *J. Chem. Ed.*, 2025, (102), 1803-1813
7. T. B. Kayyal, J. Tucker, C. M. Lowrance, L. Ajiboye, M. Pelton, J. W. Bennett, and M.-C. Daniel, “Oleic Acid Rearrangement Enables Facile Transfer of Red-Emitting Quantum

- Dots from Hexane into Water with Enhanced Fluorescence”, *Nanoscale*, 2025, (17), 12894-12910
8. A. Casale and J. W. Bennett, “Assessing the K_2BO_3 Family of Materials as Multiferroics”, *Phys. Rev. Mater.*, 2024, (8), 114424
 9. M. Layegh, P. Yan, and J. W. Bennett, “Stability of 3D and 2D materials”, *Prog. Cryst. Growth Char.*, 2024, (70), 100615
 10. A. Tauraso, G. A. Trobare, L. G. Kidd, J. E. Heimann, Z. Rosenzweig, and J. W. Bennett, “The Effects of Chlorine-Containing Species on Cinnabar: A Density Functional Theory Investigation into the Surface Adsorption Reactivity of Mercury Sulfide”, *Surf. Sci.*, 2024, (740), 122412
 11. B. G. Hudson, D. Jones, V. Rivera Bustillo, J. W. Bennett, S. E. Mason, “Understanding the mechanism of secondary cation release from the (001) surface of $Li(Ni_{1/3}Mn_{1/3}Co_{1/3})O_2$: insights from first principles”, *J. Phys. Chem. C.*, 2023, (43), 21022-21032
 12. C. S. Chari, J. E. Heimann, Z. Rosenzweig, J. W. Bennett, K. T. Faber, “Chemical Transformations of 2D Kaolinitic Clay Mineral Surfaces from Sulfuric Acid Exposure”, *Langmuir*, 2023 (39) 6964-6974
 13. J. E. Heimann, Z. Rosenzweig, and J. W. Bennett, “Understanding the Effects of Amine and Morpholine Adsorption on Unglazed Earthenware Using Density Functional Theory”, *J. Cult. Herit.*, 2023 (61) 168-176
 14. M. Layegh and J. W. Bennett, “Density Functional Theory Combined with Thermodynamics Exploration of Novel 2D Materials Created Using Aqueous Exfoliation”, *J. Phys. Chem. C.*, 2023 (127) 2314-2325
 15. R. T. Grimes and J. W. Bennett, “ Surface Transformation Thermodynamics of Alkaline Earth Carbonates Using First-Principles Calculations”, *Surface Science*, 2022 (726) 122165
 16. S. Ou, J. E. Heimann, and J. W. Bennett, “A Density Functional Theory (DFT) Investigation of Sulfur-Based Adsorbate Interactions on Alumina and Calcite Surfaces”, *Clays and Clay Minerals*, 2022 (70) 370-385
 17. J. E. Heimann, J. Tucker, L. Huff, Y.-R. Kim, J. Ali, M. K. Stroot, X. Welch, H. White, M. Wilson, C. Wood, G. Gates, Z. Rosenzweig, and J. W. Bennett, “Density Functional Theory (DFT) as a Non-Destructive Probe in the Field of Art Conservation: Small Molecule Adsorption on Aragonite Surfaces”, *ACS Appl. Mater. Inter.* 2022 (14) 13858-13871
 18. J. Dong, Y. Li, Y. Zhou, A. Schwartzmann, H. Xu, B. Azhar, J. W. Bennett, J. Li, R. Jaramillo, “Giant and Controllable Photo-Plasticity and Photo-Elasticity in Compound Semiconductors”, *Phys. Rev. Lett.* 2022 (129) 065501
 19. A. C. Khan, A. S. Cook, J. A. Leginze, and J. W. Bennett, “Developing New Antiferroelectric and Ferroelectric Oxides and Chalcogenides Within the A_2BX_3 Family” *J. Mater Res.* 2022 (37) 346-359
 20. I. K. Metz, J. W. Bennett, and S. E. Mason “Examining the Aufbau Principle and Ionization Energies: A Computational Chemistry Exercise for the Introductory Level”, *J. Chem. Ed.* 2021 (98) 4017-4025

21. J. E. Heimann, T. H. Williams, J. W. Bennett, and Z. Rosenzweig, "Baltimore SCIART: A Fully Virtual Undergraduate Research Experience at the Interface of Computational Chemistry and Art", *J. Chem. Ed.* 2021 (98) 3172-3179
22. J. E. Heimann, R. T. Grimes, Z. Rosenzweig, and J. W. Bennett, "A Density Functional Theory (DFT) Investigation of How Small Molecules and Atmospheric Pollutants Relevant to Art Conservation Adsorb on Kaolinite", *Appl. Clay Science* 2021 (206) 106075
23. J. L. Bjorklund, M. Shohel, J. W. Bennett, J. A. Smith, M. E. Carolan, E. Hollar, T. Z. Forbes and S. E. Mason, "Density Functional Theory and Thermodynamic Analysis of MA_{12} Keggin Substitution Reactions: Insights Into Ion Incorporation and Experimental Confirmation", *J. Chem. Phys.* 2021 (154) 064303
24. Ryan T. Grimes, Joshua A. Leginze, Robert Zochowski, and Joseph W. Bennett, "Surface Transformation Thermodynamics of Lead Oxides and Carbonates using First-Principles Calculations", *Inorganic Chemistry*, 2021 (60) 1228-1240
25. J. W. Bennett, "Exploring the A_2BX_3 Family for New Functional Materials using Crystallographic Database Mining and First-Principles Calculations", *J. Phys. Chem. C.*, 2020 (124) 19413-19425
26. J. W. Bennett, "Surveying Polar Materials in the Inorganic Crystal Structure Database to Identify Emerging Polar Structure Types", *J. Solid State Chem.*, 2020 (281) 121045
27. A. Abbaspour-Tamijani, J. W. Bennett, D. T. Jones, N. Cartagena-Gonzalez, Z. R. Jones, E. D. Laudadio, R. J. Hamers, J. A. Santana, S. E. Mason, "DFT and Thermodynamics Calculations of Surface Cation Release in $LiCoO_2$ ", *Appl. Surface Science*, 2020 (515) 145865
28. J. W. Bennett, D. T. Jones, B. G. Hudson, J. Melendez-Rivera, R. J. Hamers, S. E. Mason, "First-Principles and Thermodynamics Comparison of Compositionally-Tuned Delafossites: Cation Release from the (001) Surface of Complex Metal Oxides", *Environ. Sci.: Nano*, 2020 (7) 1642-1651
29. J. T. Buchman, E. A. Bennett, C. Wang, A. Abbaspour-Tamijani, J. W. Bennett, B. G. Hudson, C. M. Green, P. L. Clement, B. Zhi, A. H. Henke, E. D. Laudadio, S. E. Mason, R. J. Hamers, R. D. Klaper, C. L. Haynes, "Nickel Enrichment of Next-Generation NMC Nanomaterials Alters Material Stability, Causing Unexpected Dissolution Behavior and Observed Toxicity to *S. Oneidensis* MR-1 and *D. magna*", *Environ. Sci.: Nano*, 2020 (7) 571-587
30. J. W. Bennett, B. G. Hudson, I. Metz, D. Liang, S. Spurgeon, Q. Cui and S.E. Mason, "A Systematic Determination of Hubbard U using the GBRV Ultrasoft Pseudopotential Set", *Computational Materials Science*, 2019 (170) 109137
31. J. L. Bjorklund, J. W. Bennett, T. Z. Forbes and S. E. Mason, "Modeling of MA_{12} Keggin Heteroatom Reactivity by Anion Adsorption", *Crystal Growth & Design*, 2019 (19) 2820-2829
32. J. Bonini, J. W. Bennett, P. Chandra and K. M. Rabe, "First-Principles Bulk-Layer Model for Dielectric and Piezoelectric Responses in Superlattices", *Phys. Rev. B.*, 2019 (99) 104107

33. J. W. Bennett, M. E. Raglione, S. M. Oburn, L. M. MacGillivray, M. A. Arnold and S. E. Mason, "DFT Computed Dielectric Response and THz Spectra of Organic Co-Crystals and Their Constituent Components", *Molecules*, 2019 (24) 959
34. J. W. Bennett, X. Huang, Y. Fang, D. M. Cwiertny, V. H. Grassian and S. E. Mason, "Methane Dissociation on α -Fe₂O₃(0001) and Fe₃O₄(111) Surfaces: First-Principles Insights into Chemical Looping Combustion", *J. Phys. Chem. C.*, 2019 (123) 6450-6463
35. J. W. Bennett, D. Jones, R. J. Hamers, and S. E. Mason, "Dissolution of Compositionally-Tuned Complex Metal Oxides: A First-Principles and Thermodynamics Study of Cation Removal From the (001) Surface of Mn-rich Lithium Nickel Manganese Cobalt Oxide", *Inorg. Chem.*, 2018 (57) 13300-13311
36. E. D. Laudadio, J. W. Bennett, C. M. Greene, S. E. Mason and R. J. Hamers, "Impact of Phosphate Adsorption on Complex Lithium Cobalt Oxide Nanoparticle Dispersibility in Aqueous Media", *Environ. Sci. Technol.*, 2018 (52) 10186-10195
37. J. W. Bennett, D. Jones, X. Huang, R. J. Hamers and S. E. Mason, "The Dissolution of Complex Metal Oxides from First-Principles and Thermodynamics: Cation Removal from the (001) Surface of Li(Ni_{1/3}Mn_{1/3}Co_{1/3})O₂", *Environ. Sci. Technol.*, 2018 (52) 5792-5802
38. D. Liang, J. Hong, D. Fang, J. W. Bennett, S. E. Mason, R. J. Hamers and Q. Cui, "Analysis of Conformational Properties of Amine Ligands at the Gold/Water Interface with QM, MM, and QM/MM simulations", *Phys. Chem. Chem. Phys.*, 2018 (20) 3349-3362
39. J. W. Bennett, J. L. Bjorklund, T. Z. Forbes and S. E. Mason, "A Survey of the Reactivity Relationships of Anionic Adsorbates on Aluminum Nanoclusters", *Inorg. Chem.*, 2017 (56) 13014-13028
40. X. Huang, J.W. Bennett, M. N. Hang, E. D. Laudadio, R. J. Hamers, and S. E. Mason, "Ab initio Atomistic Thermodynamics Study of the (001) Surface of LiCoO₂ in a Water Environment and Implications for Reactivity under Ambient Conditions", *J. Phys. Chem. C.*, 2017 (121) 5069-5080
41. B. Monserrat, J. W. Bennett, K. M. Rabe, and D. Vanderbilt, "Antiferroelectric topological insulators in ABC compounds", *Phys. Rev. Lett.*, 2017 (119) 036802
42. I. L. Gunsolus, M. N. Hang, N. V. Hudson-Smith, J. Buchman, J. W. Bennett, D. Conroy, S. E. Mason, C. Haynes and R. Hamers, "Influence of Nickel Manganese Cobalt Nanoparticle Composition on Toxicity Toward *Shewanella Oneidensis* MR-1: Redesigning for Reduced Biological Impact", *Environ. Sci.: Nano*, 2017 (4) 636-646
43. K. W. Corum, X. Huang, J. W. Bennett and S. E. Mason, "Systematic Density Functional Theory Study of the Structural and Electronic Properties of Constrained and Fully Relaxed (001) Surfaces of Alumina and Hematite", *Molec. Simul.* 2017 (43) 406-419
44. K. F. Garrity, J. W. Bennett, K. M. Rabe and D. Vanderbilt, "Pseudopotentials for high-throughput DFT calculations", *Comp. Mater. Sci.*, 2014, (81), 446
45. J. Brehm, J. W. Bennett, M. R. Schoenberg, I. Grinberg, and A. M. Rappe, "The structural diversity of ABS₃ compounds with d⁰ electronic configuration for the B-cation", *J. Chem. Phys.*, 2014 (140) 224703-1-8

46. J. A. Brehm, H. Takenaka, C.-W. Lee, I. Grinberg, J.W. Bennett, M. R. Schoenberg, and A. M. Rappe, "Density functional theory study of PbTiO₃-based oxysulfides", *Phys. Rev. B.*, 2014 (89) 195202-1-8
47. J. W. Bennett, K. F. Garrity, K. M. Rabe, D. Vanderbilt, "Orthorhombic *ABC* semiconductors as antiferroelectrics", *Phys. Rev. Lett.*, 2013, (110), 017603
48. J. W. Bennett and K.M. Rabe, "Integration of first-principles methods and crystallographic database searches for new ferroelectrics: Strategies and explorations", *J. Solid State Chem.*, 2012, (195) 21-31
49. J. W. Bennett, K. F. Garrity, K. M. Rabe and D. Vanderbilt, "Hexagonal *ABC* semiconductors as ferroelectrics", *Phys. Rev. Lett.*, 2012, (109) 167602
50. A. Roy, J. W. Bennett, K. M. Rabe and D. Vanderbilt, "Half-Heusler semiconductors as piezoelectrics", *Phys. Rev. Lett.* 2012, (109) 037602
51. T. Qi, M. T. Curnan, S. Kim, J. W. Bennett, I. Grinberg and A. M. Rappe, "A first-principles study of band gap engineering via oxygen vacancy doping in *ABB'*O₃ perovskite solid solutions", *Phys. Rev. B.*, 2011, (84), 245206
52. G. Y. Gou, J. W. Bennett, H. Takenaka and A. M. Rappe, "Post density functional theory studies of highly polar semiconductor PbTi_{1-x}Ni_xO_{3-z} solutions", *Phys. Rev. B.*, 2011, (83) 205115-1-7
53. J. W. Bennett, I. Grinberg, P. K. Davies and A. M. Rappe, "Pb-free ferroelectrics investigated with density-functional theory: Sn(Al_{1/2}Nb_{1/2})O₃ perovskites", *Phys. Rev. B.*, 2011, (83) 144122-1-6
54. J. W. Bennett, I. Grinberg, P. K. Davies and A. M. Rappe, "Pb-free semiconductor ferroelectrics: A theoretical study of Pd-substituted Ba(Ti_{1-x}Ce_x)O₃ solid solutions", *Phys. Rev. B*, 2010, (82) 184106-1-5
55. J. W. Bennett, I. Grinberg and A. M. Rappe, "The effect of substituting S for O: The sulfide perovskite BaZrS₃", *Phys. Rev. B.*, 2009, (79) 235115-1-6
56. J. W. Bennett, I. Grinberg and A. M. Rappe, "New highly polar semi-conductor ferroelectrics through *d*⁸-cation O-vacancy doping of PbTiO₃", *J. Amer. Chem. Soc.*, 2008, (130), 17409-17412
57. J. W. Bennett, I. Grinberg and A. M. Rappe, "Non-monotonic composition dependence of the dielectric response of Ba_{1-x}Ca_xZrO₃", *Chem. Mater.*, 2008, (20), 5134-5138
58. J. Li, U. G. Singh, J. W. Bennett, K. Page, J. Weaver, J. P. Zhang, T. Proffen, A. M. Rappe, S. L. Scott and R. Seshadri, "BaCe_{1-x}Pd_xO₃ : Redox controlled ingress and egress of palladium in a perovskite", *Chem. Mater.*, 2007, (19), 1418-1426
59. U. G. Singh, J. Li, J. W. Bennett, A. M. Rappe, R. Seshadri and S. L. Scott, "A Pd-doped perovskite catalyst, BaCe_{1-x}Pd_xO_{3-z}, for CO oxidation", *J. Catalysis*, 2007, (249), 349-358
60. J. W. Bennett, I. Grinberg and A.M. Rappe, "Effect of symmetry-lowering on the dielectric response of BaZrO₃", *Phys. Rev. B.*, 2006, (73), 180102(R)
61. S. Solomon, B. Brook, S. Rutkowsky and J. Bennett, "Using ice-cooled condensers in chemistry laboratory", *J. Chem. Ed.*, 2003, (80), 299-301

Non-Peer-Refereed Works

Articles

1. J. W. Bennett, C. Allen, S. Pramanik, M. J. Gallagher, N. V. Hudson-Smith, D. Jones, M. O. P. Krause and S. E. Mason, "Research highlights: comparing the biological response of nanoparticle solid solutions", *Environ. Sci.: Nano*, 2017 (4) 1428-1432

Conference Proceedings

2. J. W. Bennett, "Discovery and design of functional materials: Integration of database searching and first-principles calculations", *Physics Procedia*, 2012, (34) 14-23
3. T. Qi, J. W. Bennett, W. Al-Saidi, I. Grinberg and A. M. Rappe, "Studies of perovskite materials for high performance piezoelectrics and non-volatile memory", *IEEE Proceedings*, 2011, DoD HPCMP UGC 459-469
4. T. Qi, I. Grinberg, J. W. Bennett, Y. H. Shin, A. M. Rappe, K. L. Yeh and K. A. Nelson, "Studies of perovskite materials for high-performance storage media, piezoelectric, and solar energy conversion devices", *IEEE Proceedings*, 2010, DoD HPCMP UGC 249-258
5. T. Qi, S. V. Levchenko, J. W. Bennett, I. Grinberg and A. M. Rappe, "New Prospects for High-Performance SONAR, Chemical Sensor and Communication Device Materials", *IEEE Proceedings*, 2009, DoD HPCMP UGC, 197-204
6. J. W. Bennett, I. Grinberg, Y. H. Shin and A. M. Rappe, "Modeling of materials for naval SONAR, pollution control and non-volatile memory application", *IEEE Proceedings*, 2008, DoD HPCMP UGC, 214-220

PRESENTATIONS

Invited Seminars

1. J. W. Bennett, "Database-Driven Discovery of New Ferroics using First-Principles Methods", Johns Hopkins University Department of Chemistry, Baltimore, MD, March 2026
2. J. W. Bennett, "Database-Driven Discovery of New Ferroics using First-Principles Methods", Drexel University Department of Materials Science and Engineering, Philadelphia, PA, Nov 2025
3. J. W. Bennett, "Teaching About Surfaces at the Interface of Chemistry and Computing in STEM", Penn Conference on Theoretical Chemistry, University of Pennsylvania, Philadelphia, PA, May 2025
4. J. W. Bennett, "Modeling of Thin Film Growth on 2D Materials", CFN at Brookhaven National Lab, Upton, NY, April 2025
5. J. W. Bennett, "The Discovery and Design of New Materials as Multifunctional Platforms", Rutgers Newark Department of Physics, Newark, NJ, November 2024
6. J. W. Bennett, "The Discovery and Design of New Materials as Multifunctional Platforms", Lebanon Valley College Department of Chemistry, Lebanon, PA, November 2024
7. J. W. Bennett, "The Discovery and Design of New Materials as Multifunctional Platforms", Carnegie Mellon Department of Chemical Engineering, Pittsburgh, PA, October 2024
8. J. W. Bennett, "The Discovery and Design of New Materials as Multifunctional Platforms", Cornell University Department of Materials Science and Engineering, Ithaca, NY, September 2024
9. J. W. Bennett, "The Discovery and Design of New Materials as Multifunctional Platforms", Virginia Tech Department of Chemistry, Blacksburg, VA, October 2023
10. J. W. Bennett, "The Discovery and Design of New Materials as Multifunctional Platforms", Coppin State University, Baltimore, MD, May 2023

11. J. W. Bennett, "The Discovery and Design of New Materials as Multifunctional Platforms", University of Maryland College Park MSE, College Park, MD, May 2023
12. J. W. Bennett, "Density Functional Theory (DFT) as a Noninvasive Probe in the Field of Art Conservation Science", Millersville University, Millersville PA, September 2022
13. J. W. Bennett, "Density Functional Theory (DFT) as a Noninvasive Probe in the Field of Art Conservation Science", Lehigh Valley ACS Meeting, April 2022
14. J. W. Bennett, "Search for New Piezoelectrics, Ferroelectrics, and Antiferroelectrics", UMBC Department of Physics Colloquium, Baltimore, MD, December 2020
15. J. W. Bennett, "Atomistic Insights into Safer Water and Cleaner Energy", UMBC Department of Chemistry and Biochemistry, Baltimore, MD, November 2020
16. J. W. Bennett, "Thermodynamics of Complex Metal Oxide Surface Transformations", UMBC Department of Chemistry and Biochemistry, Baltimore, MD, USA, January 2019
17. J. W. Bennett, "DFT Methods for Modeling Nanomaterials", Tuskegee University Department of Chemistry, Tuskegee, AL, USA, September 2017
18. J. W. Bennett, "The Search for New Functional Materials: New Classes of Piezoelectrics, Ferroelectrics, and Antiferroelectrics", University of Iowa Department of Chemistry, Iowa City, IA, USA, March 2016
19. J. W. Bennett, "The Search for New Functional Semiconductors", Naval Research Laboratory Electronics Science and Technology Division, Washington, D.C., USA, October 2015
20. J. W. Bennett, "Discovery and Design of Multifunctional Materials", Laboratory for Surface Modification Seminar, Rutgers University, Piscataway, NJ, USA, April 2012
21. J. W. Bennett, "Discovery and Design of Multifunctional Materials", Argonne National Lab Materials Science Division, Argonne, IL, USA March 2012
22. J. W. Bennett, "Identifying Pb-free Multifunctional Materials", University of Iowa Department of Chemistry, Iowa City, IA, USA, July 2011

Invited Oral Presentations at National/International Conferences (Juried/Refereed)

23. J. W. Bennett, "The Rational Design of New Antiferroelectrics and Ferroelectrics for Energy Applications" American Chemical Society Mid-Atlantic Regional Meeting, TCNJ, Trenton, NJ, June 2022
24. J. W. Bennett, "Designing New Functional Semiconductors from First-Principles", Materials Research Society Spring Meeting, online, April 2021
25. (J. W. Bennett), S. E. Mason*, "DFT Methods for Solid-Liquid Interfaces", CECAM Workshop on Tackling Complexity of the Nano-Bio Interface, Bremen University, Bremen, Germany, June 2017
26. (J. W. Bennett), K. M. Rabe*, "New Ferroelectrics and Antiferroelectrics by Design", 7th International Conference on Electroceramics, Penn State University, State College, PA, USA, May 2015
27. J. W. Bennett, "New Classes of Piezoelectrics, Ferroelectrics, and Antiferroelectrics by First-Principles High-Throughput Materials Design", March Meeting of the American Physical Society, Baltimore, MD, USA, March 2013
28. J. W. Bennett, "New Classes of Piezoelectrics, Ferroelectrics, and Antiferroelectrics by First-Principles High-Throughput Materials Design", 16th Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, Abdus Salam International Center for Theoretical Physics, Trieste, Italy, January 2013
29. J. W. Bennett, "Integration of Database Mining and First-Principles Calculations: Discovery and Design of Multifunctional Materials", 24th Annual Electronic Structure Workshop, Wake Forest University, Winston-Salem, NC, USA, June 2012
30. J. W. Bennett, "Discovery and Design of Functional Materials: Integration of Database

Searching and First-Principles Calculations”, Center for Simulation Physics Workshop at the University of Georgia, Athens, GA, USA, February 2012

Oral Presentations at National/International Conferences (Juried/Refereed)

1. J. W. Bennett*, “Data-Driven Assessment of Modeling 2D van der Waals Materials with Homonuclear Bonds”, Materials Research Society Fall Meeting, Boston, MA, December 2025
2. J. W. Bennett*, “Training the Next Generation of Computational Materials Scientists with Open Source DFT Calculations of Electronic Band Structure”, Materials Research Society Fall Meeting, Boston, MA, December 2025
3. (P. Yan), J. W. Bennett*, “Data-Enabled Discovery of Two-Dimensional van der Waals Layered Phosphochalcogenides”, Materials Research Society Fall Meeting, Boston, MA, December 2025
4. (A. Casale), J. W. Bennett*, “Evaluating Magnetic Moment Support in A_2BO_3 Systems”, Materials Research Society Fall Meeting, Boston, MA, December 2025
5. (A. Casale), J. W. Bennett*, “Assessing the K_2BO_3 Family of Materials as Multiferroics”, American Chemical Society Fall Meeting, Washington, D.C., August 2025
6. (P. Yan), J. W. Bennett*, “Homonuclear Bonds and Their Impact on the Functional Properties of 2D Layered van der Waals Materials,” Materials Research Society Spring Meeting, Seattle, WA, April 2025
7. (M. Layegh), J. W. Bennett*, “ ΔG -Driven Surface Transformations in 2D Material Formation: DFT Insights to Inform Future Data-Driven Models,” Materials Research Society Spring Meeting, Seattle, WA, April 2025
8. (A. Casale), J. W. Bennett*, “First-Principles Analysis of Transition Metal Nitrates in Oxide Host Sensor Materials”, Chemical and Biological Defense Science and Technology Conference, Ft. Lauderdale, FL, December 2024
9. (P. Yan), J. W. Bennett*, “Implications for Corrosion Inhibition of Electrochemical Interfaces through Atomistic Insights into Phosphate Thin Film Growth on Lead-Containing Materials,” Materials Research Society Spring Meeting, Boston, MA, November 2024
10. J. W. Bennett*, “Teaching Density Functional Theory to Students of Art Conservation,” American Chemical Society Fall Meeting, Denver, CO, August 2024
11. J. W. Bennett*, “Using Inorganic Chemistry to Design New Functional Semiconductors with a Computer,” American Chemical Society Fall Meeting, Denver, CO, August 2024
12. J. W. Bennett*, “Data-Enabled Discovery and Design of New Multiferroic Materials,” Solid State Chemistry Gordon Research Conference, Colby College, NH, July 2024
13. J. W. Bennett*, “Teaching Density Functional Theory to Students of Art Conservation,” Materials Research Society Spring Meeting, Seattle, WA, April 2024
14. J. W. Bennett*, “Using Inorganic Chemistry to Design New Functional Semiconductors with a Computer,” Materials Research Society Spring Meeting, Seattle, WA, April 2024
15. J. W. Bennett*, “The Discovery and Design of New Ferroic A_2BX_3 Materials,” Fundamental Physics of Ferroelectrics, Washington, D.C., February 2024
16. (P. Yan), J. W. Bennett*, “Interfacial Adsorption and Growth of Phosphates on Lead Oxide and Carbonate Microcontaminants in Aqueous Environments,” American Chemical Society Fall Meeting, San Francisco, CA, August 2023
17. (A. Casale), J. W. Bennett*, “Data Enabled Design of Multiferroics in the A_2BX_3 Family of Materials”, American Chemical Society Fall Meeting, San Francisco, CA, August 2023

18. (M. Layegh), J. W. Bennett*, “Eco-friendly Synthesis of Novel 2D Materials Using DFT and Thermodynamics,” American Chemical Society Fall Meeting, San Francisco, CA, August 2023
19. J. W. Bennett, “Design and Discovery of Solid State Ferroelectrics and Antiferroelectrics”, American Chemical Society Fall Meeting, San Francisco, CA, August 2023
20. J. W. Bennett, “Combining Online Resources and First-Principles Modeling to Design New Functional Materials”, American Chemical Society Fall Meeting, San Francisco, CA, August 2023
21. (A. Casale), J. W. Bennett*, “Designed Multiferroics in the A_2BX_3 Family of Materials”, American Chemical Society Spring Meeting, held online, April 2023
22. (A. Tauraso), G. A. Trobare, J. W. Bennett*, “First-Principles Calculations as a Noninvasive Probe of Vermillion and Cinnabar Surfaces in Art Conservation Science”, American Chemical Society Spring Meeting, held online, April 2023
23. (G. A. Trobare), A. Tauraso, J. W. Bennett*, “First-Principles Calculations as a Noninvasive Probe of Vermillion and Cinnabar Surfaces in Art Conservation Science”, American Chemical Society Spring Meeting, held online, April 2023
24. (L. Kidd), G. Trobare, A. Tauraso, J. W. Bennett*, “A Noninvasive Computational Investigation of the Photodegradation of Vermillion”, ABRCMS Anaheim, CA, November 2022
25. (M. Layegh), J. W. Bennett*, “Designing New 2D Nanomaterials with an Environmentally Friendly Synthesis Route: A DFT + Solvent Ion Model Driven Study”, Fall MRS Meeting, Boston, MA, November 2022
26. J. W. Bennett, “First-Principles Density Functional Theory as a Noninvasive Probe to Understand the Surface Transformations of Minerals Important to Cultural Heritage”, Gordon Research Conference on Scientific Methods in Cultural Heritage Research, Les Diablerets, July 2022
27. J. W. Bennett, “Delineating the Thermodynamics of Carbonate Dissolution in Aqueous Media by Combining First-Principles and Experiments”, American Chemical Society Spring Meeting, held online, March 2022
28. J. W. Bennett, “The Rational Design of New Antiferroelectrics and Ferroelectrics”, Materials Research Society, held online, May 2022
29. (J. Tucker), J. E. Heimann, Z. Rosenzweig, J. W. Bennett*, “What Damages the Aragonite Artifacts in Museums? A First-Principles Survey of $CaCO_3$ Surface Adsorption Reactivity”, American Chemical Society Spring Meeting, held online, March 2022
30. (A. Casale), J. W. Bennett*, “Data-Enabled Search Methods to Design New Polar Metals”, American Chemical Society Spring Meeting, held online, March 2022
31. (M. Layegh), J. W. Bennett, “Surface Reactivity of 2D Nanomaterials in Water Using a DFT + Thermodynamics Framework”, American Chemical Society Spring Meeting, held online, March 2022
32. (A. Khan), J. W. Bennett*, “Computational Discovery of New Functional Materials for Energy Generation and Storage”, American Chemical Society Spring Meeting, held online, March 2022
33. (J. E. Heimann), J. W. Bennett, Z. Rosenzweig*, Baltimore SCIART Program: Undergraduate Research in Utilizing Density Functional Theory (DFT) as a Non-Destructive Probe in the Field of Art Conservation”, American Chemical Society Spring Meeting, held online, March 2022
34. J. W. Bennett, “Designing New Functional Semiconductors from First Principles”, American Chemical Society Spring Meeting, held online, April 2021

35. (J. E. Heimann), T. Williams, J. W. Bennett, Z. Rosenzweig*, “Baltimore SCIART: A Fully Virtual Undergraduate Research Experience at the Interface of Computational Chemistry and Art”, American Chemical Society Spring Meeting, held online, April 2021
36. (M. Layegh), J. W. Bennett*, “First-Principles Insights into the Chemical Manipulation of 3D Solids to Create New 2D Materials”, American Chemical Society Spring Meeting, held online, April 2021
37. (J. A. Leginze), J. W. Bennett*, “Use of Density Functional Theory and First-Principles Thermodynamics in Understanding Lead Oxide Surface Transformations”, American Chemical Society Spring Meeting, held online, April 2021
38. (A. S. Cook), J. W. Bennett*, “Discovering and Characterizing New Functional Ferroelectric and Antiferroelectric Materials Using Computers”, American Chemical Society Spring Meeting, held online, April 2021
39. (R. T. Grimes), J. W. Bennett*, “First-principles Modeling of Lead Dissolution Thermodynamics in PbCO_3 ”, American Chemical Society Spring Meeting, held online, April 2021
40. (A. Khan), J. W. Bennett*, “Systematic Route to Explore the Potential Energy Landscape of a New Family of Functional Materials”, American Chemical Society Spring Meeting, held online, April 2021
41. (J. Heimann), J. W. Bennett, Z. Rosenzweig*, “Adsorption on Kaolinite Surfaces: A Density Functional Theory (DFT) Approach to Quantifying Interactions Between a Clay Mineral and Small Molecules,” Eastern Analytical Symposium & Exposition, Virtual, USA, November 2020
42. (J. Heimann), J. W. Bennett, Z. Rosenzweig*, “Adsorption on Kaolinite Surfaces: A Density Functional Theory (DFT) Approach to Quantifying Interactions Between a Clay Mineral and Small Molecules,” Materials Science and Technology, Virtual, USA, November 2020
43. J. W. Bennett*, “Combining Database Mining and DFT to Create New Materials”, American Chemical Society Meeting, Philadelphia, PA, USA, March 2020 (*posted online)
44. (J. W. Bennett), S. E. Mason*, “Thermodynamics of Cation Dissolution from Complex Metal Oxides”, American Chemical Society Meeting, New Orleans, LA, USA, March 2018
45. J. W. Bennett*, “Polar Compounds with Desirable Properties: Identifying New Functional Materials”, American Chemical Society Meeting, Philadelphia, PA, USA, August 2016
46. (J. W. Bennett), K. M. Rabe*, “Semiconductive Hexagonal ABC as Ferroelectrics”, Materials Research Society Spring Meeting, San Francisco, CA, USA, April 2012
47. (J. W. Bennett), K. M. Rabe*, “The Search for Multifunctional Polar Materials”, American Physical Society Meeting, Dallas, TX, USA, March 2011
48. (J. W. Bennett), K. M. Rabe*, “The Search for Multifunctional Polar Materials”, Ferroelectrics Workshop, Gaithersburg, MD, USA February 2011
49. (J. W. Bennett), K. M. Rabe*, “The Search for Multifunctional Polar Materials”, Materials Research Society Fall Meeting, Boston, MA, USA, November 2010
50. (J. W. Bennett), A. M. Rappe*, “New Highly Polar Semiconductor Ferroelectrics for Solar Conversion”, American Physical Society Meeting, Pittsburgh, PA, USA, March 2009
51. (J. W. Bennett), A. M. Rappe*, “First-Principles Modeling of $\text{Ba}(\text{Ce}, \text{Pd})\text{O}_3$: Redox,

- Structure, and Chemistry”, American Chemical Society Meeting, New Orleans, LA, USA, April 2008
52. (J. W. Bennett), A. M. Rappe*, “First-Principles Modeling of BaCeO₃: Stabilization of O-vacancies”, American Physical Society Meeting, New Orleans, LA, USA, March 2008
 53. (J. W. Bennett), A. M. Rappe*, “DFT Models as a Way to Study Pd-doped BaCeO₃”, Ferroelectrics Workshop, Williamsburg, VA, USA, February 2007
 54. (J. W. Bennett), A. M. Rappe*, “A First-Principles Approach to Modeling (Ba,Ca)ZrO₃”, American Physical Society Meeting, Baltimore, MD, USA, March 2006

Oral Presentations at Regional Conferences/Symposia (Juried/Refereed)

55. (A. Tauraso), J. W. Bennett*, “The Effects of Chlorine-Containing Species on Cinnabar: A Density Functional Theory Investigation on the Surface Adsorption Reactivity of Mercury Sulfide,” LSAMP 2023, College Park MD, USA, December 2023
56. (A. Khan), J. W. Bennett*, “Computational Discovery of New Functional Materials for Energy Generation and Storage, LSAMP 2021, College Park MD, USA, December 2021
57. (J. W. Bennett), S. E. Mason*, “Thermodynamics of Complex Metal Oxide Transformations”, Midwest Theoretical Chemistry Conference”, University of Chicago, Chicago, IL, USA, June 2018
58. (J. W. Bennett), S. E. Mason*, “Modeling the Dissolution of Complex Metal Oxide Cathode Materials”, ACS-MWRM, Kansas State University, Manhattan, KS, USA, October 2016

Oral Presentations at Regional Conferences/Symposia (Non-Juried/Non-Refereed)

1. J. W. Bennett*, “Open-Source DFT Calculations to Understand Bonding in Solids”, Amazing Chemistry Insights and Discussions (ACID) Series, Penn State Berks (virtual), Berks, PA, August 2025
2. (K. Schwanebeck), Zeev Rosenzweig, J. W. Bennett*, “First-Principles Investigation of Ti₃T₂C₂ MXene with Small Molecule Adsorbates (T=O, F, H, OH)”, UMBC SURF, August 2025
3. (B. Webb), Zeev Rosenzweig, J. W. Bennett*, “Analysis of Surface Transformations and Electronic States of Oxygen, Hydrogen, Fluoride, and Hydroxide Terminated MXenes”, UMBC SURF, August 2025
4. (M. Layegh), J. W. Bennett*, “Open-Source DFT Calculations to Understand Bonding in Solids” UMBC Chemistry & Biochemistry Graduate Research Day, Baltimore, MD, March 2025
5. (P. Yan), J. W. Bennett*, “2D Hybrid Organic-Inorganic Platforms” UMBC Chemistry & Biochemistry Graduate Research Day, Baltimore, MD, March 2025
6. (A. Casale), J. W. Bennett*, “DFT Analysis Methods of 2D van der Waals Materials” UMBC Chemistry & Biochemistry Graduate Research Day, Baltimore, MD, March 2025
7. (O. Chiarini, C. Doherty), J. W. Bennett, Z. Rosenzweig*, “2D MXenes as Chemical Sensors in the Art Museum Environment”, UMBC SURF, August 2024
8. (R. Smith), J. W. Bennett*, “Data-Enabled Computational Chemistry to Better Understand Water Quality”, UMBC URCAD, April 2024

9. (M. Liu), J. W. Bennett*, “Ferroelectrics Designed Using A-site Ion Substitution in Hexagonal $AZnSb$ ”, UMBC URCAD, April 2024
10. (P. Yan), J. W. Bennett*, “Computational Simulation of Thin Film Growth of Phosphate Corrosion Inhibitor on Lead-Containing Materials in Water” UMBC Chemistry & Biochemistry Graduate Research Day, Baltimore, MD, April 2024
11. (M. Layegh), J. W. Bennett*, “Unveiling Novel 2D Materials: DFT and Thermodynamics Analysis” UMBC Chemistry & Biochemistry Graduate Research Day, Baltimore, MD, April 2024
12. (A. Casale), J. W. Bennett*, “Multiferroic Structures in the A_2BX_3 Family of Materials” UMBC Chemistry & Biochemistry Graduate Research Day, Baltimore, MD, April 2024
13. (R. Smith), J. W. Bennett*, “Data-Enabled Computational Chemistry to Better Understand Water Quality”, UMBC SURF, August 2023
14. (C. Doherty, J. Ngo), J. E. Heimann, J. W. Bennett, Z. Rosenzweig*, “The Impact of Nitrates and Phosphates on the Surface of Calcite: First-Principles Analysis of Calcium Carbonate”, UMBC SURF, August 2023
15. (J. Birenzvige), J. E. Heimann, J. W. Bennett, Z. Rosenzweig*, “An Ab Initio Investigation of Various Sulphates on a Calcite Surface Using Density Functional Theory”, UMBC SURF, August 2023
16. (R. Rehling), J. E. Heimann, J. W. Bennett, Z. Rosenzweig*, “The Impact of Chlorides on the Surface of Calcite: A Density Functional Theory Analysis of Calcium Carbonate” UMBC SURF, August 2023
17. (J. Birenzvige), J. W. Bennett*, “Phosphochalcogenides as Tunable Ferroelectrics”, UMBC URCAD, Baltimore, MD, April 2023
18. (A. Tauraso), J. W. Bennett*, “Adsorption Reactivity and Electronic Band Structure Analysis of Vermillion Surfaces in Art Conservation Science”, UMBC URCAD, Baltimore, MD, April 2023
19. (G. A. Trobare), J. W. Bennett*, “First-Principles Calculations as a Noninvasive Probe of Vermillion and Cinnabar Surfaces in Art Conservation Science”, UMBC URCAD, Baltimore, MD, April 2023
20. (A. Casale), J. W. Bennett*, “Multiferroic Structures in the A_2BX_3 Family of Materials” UMBC Chemistry & Biochemistry Graduate Research Day, Baltimore, MD, April 2023
21. (M. Layegh), J. W. Bennett*, “Unveiling Novel 2D Materials: DFT and Thermodynamics Analysis” UMBC Chemistry & Biochemistry Graduate Research Day, Baltimore, MD, April 2023
22. (P. Yan), J. W. Bennett*, “Computational Simulation of Thin Film Growth of Phosphate Corrosion Inhibitor on Lead-Containing Materials in Water” UMBC Chemistry & Biochemistry Graduate Research Day, Baltimore, MD, April 2023
23. (A. Tauraso, G. A. Trobare, L. Kidd), J. E. Heimann, Z. Rosenzweig, J. W. Bennett*, “A Noninvasive Computational DFT Investigation of the Photodegradation of Vermillion”, UMBC SURF, August 2022, online
24. (A. Khan), J. W. Bennett*, “Computational Discovery of New Functional Materials for Energy Generation and Storage”, UMBC URCAD, April 2022, online

25. (M. Layegh), J. W. Bennett*, “Surface Reactivity of 2D Nanomaterials in Water Using a DFT + Thermodynamics Framework” UMBC Chemistry & Biochemistry Graduate Research Day, Baltimore, MD, April 2022
26. (A. Casale) J. W. Bennett*, “Data-Enabled Search Methods to Design New Polar Metals” UMBC Chemistry & Biochemistry Graduate Research Day, Baltimore, MD, April 2022
27. (M. Layegh) J. W. Bennett*, “First-Principles Insights into the Chemical Manipulation of 3D Solids to Create New 2D Materials” UMBC Chemistry & Biochemistry Graduate Research Day, April 2021, online.
28. (A. Khan), J. W. Bennett*, “Systematic Route to Explore the Potential Energy Landscape of a New Family of Functional Materials”, UMBC URCAD, April 2021, online.
29. (A. S. Cook), J. W. Bennett*, “Discovering and Characterizing New Functional Ferroelectric and Antiferroelectric Materials Using Computers”, UMBC URCAD, April 2021, online.
30. (J. A. Leginze), J. W. Bennett*, “Use of Density Functional Theory and First-Principles Thermodynamics in Understanding Lead Oxide Surface Transformations”, UMBC URCAD, April 2021, online.

SERVICE

Departmental activities

- Winter 2024 – present Science Olympiad (Geologic Mapping, 2x Materials Science C)
- Spring 2022 – present Member of the Departmental Website Committee
- Fall 2021 – present Co-Chair of the Departmental Seminar Committee
- Winter 2021 – present Computational Advisor to Sci-Art Program, run 7x
- Fall 2020 - present Member of the Graduate Student Recruiting Committee
- Spring 2020 Poster Session Judge at the Graduate Research Symposium
- Fall 2019- present Presented Research Overview to 1st Year UMBC Chemistry Graduate Students during Summer Bridge, 7x

List of other PhD Students Committees served/serving on

Ayden Roberts	degree expected in 2030
Codi Hrynko	degree expected in 2030
Jeanne Ngo	degree expected in 2030
Emmanuella Duruye	degree expected in 2029
Durga Devkota	degree expected in 2028
Lekan Ajiboye	degree expected in 2027
Aminah Amjad	degree expected in 2026
Leopoldo Posada-Escobar	degree expected in 2025
Alexander Paredes	degree expected in 2025
Mark Gabriana	degree awarded in 2024
Shreyasi Sengupta	degree awarded in 2024
Chanda Lowrance	degree awarded in 2024

Alex Sestok degree awarded in 2022

University activities

- Fall 2024-present Member of the Shared Infrastructure Governance Advanced CPU Committee for UMBC HPCF
- April 2023 Served as a Judge for the 3 Minute Thesis Competition
- Spring 2023 – Fall 2024 Member of the Research Computing Task Force
- September 2022 Retriever Recruitment
- Fall 2020 – Fall 2024 Member of the High-Performance Computing Facility Governance Committee
- Fall 2019 Served as Judge for UMBC Undergraduate Research Symposia
- Fall 2019 - present Member of the LGBTQ Faculty Staff Association
- Fall 2019 Installed and tested open source codes for student research use on UMBC HPCF machines

Professional activities

Affiliations:

- 2004 – Present American Chemical Society
- 2010 – Present Materials Research Society
- 2023 – Present NSF Panelist (January 2023, May 2023, ad hoc)
- 2024 – Present User Executive Committee Member of CFN at Brookhaven

Panelist: 2024 MRS AIChE Pride Month Webinar Panelist

Ad Hoc Proposal Review for National Science Foundation DMR and Department of Energy

Proposal Review for GUP allocations from CFN Theory and Computing (2023-present, 4x year)

Ad Hoc Manuscript Review for:

- *Science*
- *Physical Review B*
- *Journal of Vacuum Science and Technology B*
- *Nature Communications*
- *APL Materials*
- *Applied Physics Letters*
- *Accounts of Chemical Research*
- *J. Phys. Chem. C.*
- *Ceramics International*
- *Physical Review Letters*
- *Physical Review Materials*
- *Computational Materials Science*
- *Journal of Solid State Chemistry*
- *New Journal of Chemistry*

I certify that this document is accurate and true.

Joseph W. Bennett

A handwritten signature in black ink, appearing to read 'Joseph W. Bennett', is centered on a light gray rectangular background.

November 26, 2025