

## **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**

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

## **Experience in Other Than Higher Education**

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

## **Honors and Awards**

2021	UMBC START grant FY21
2019-2021	UMBC 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**

- 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-	“Designing Multiferroic Composites from Layered Ferroelectric Chalcogenides and van der Waals Ferromagnets” <u>source</u> : DTRA, <u>role</u> : co-PI, <u>amount</u> : \$750,000
2019 –2023	“Atomistic Insights into Safer Water and Cleaner Energy from Density Functional Theory”, <u>source</u> : NSF-XSEDE, <u>role</u> : PI, <u>amount</u> : 1.200,000+ SU
2022	“DFT Methods as a Noninvasive Probe for Art Conservation Science in the Baltimore SCIART Summer Program”, <u>source</u> : NSF-XSEDE, <u>role</u> : PI, <u>amount</u> : 50,000 SU
2020 – 2021	Recipient of FY21 START grant, <u>source</u> : UMBC, <u>role</u> : PI, <u>amount</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</u> : \$10,000

### **Ph.D. Students**

- Mona Layegh, degree expected in 2024, Role: PhD advisor/committee Chair
- Anthony Casale, degree expected in 2025, Role: PhD advisor/committee Chair
- Peng Yan, degree expected in 2026, Role: PhD advisor/committee Chair

### **Undergraduate Students**

- Rachel Rehling, UMBC undergraduate research (June 2023-December 2023), Role: research mentor
- Rayal Smith, UMBC undergraduate research & LSAMP scholar (June 2023-present), Role: research mentor
- Joshua Birenzvice, UMBC undergraduate research (December 2022-May 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-present), Role: research mentor
- Eunice Costanzo, Merck Undergraduate Fellow & UMBC undergraduate research (May 2022-May 2023), degree expected in 2023, 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**

- Skye Eliot, Blair Montgomery High School 2022-present, *Role:* research mentor
- Stanley Ou, Blair Montgomery High School 2021, Role: research mentor

### **Student Awards**

- Anthony Casale, Army Education Outreach Program (\$74,800), Sept 2023-Sept 2024
- 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. M. Layegh, P. Yan, and J. W. Bennett, “Stability of 3D and 2D materials”, *Prog. Cryst. Growth Char., in preparation* (9/2023)
2. T. B. Kayyal, J. Tucker, C. M. Lowrance, M. Pelton, J. W. Bennett, and M.-C. Daniel, “Doubling Photoluminescence Quantum Yield of Bright, Red-Emitting Quantum Dots in Water through Facile Transfer from Hexane without any Additional Reagents”, *submitted* (9/2023)
3. 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, *in revision* (8/2023)
4. 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  $\text{Li}(\text{Ni}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3})\text{O}_2$ : insights from first principles”, *J. Phys. Chem. C., in revision*, (8/2023)
5. 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
6. 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
7. 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
8. R. T. Grimes and J. W. Bennett, “Surface Transformation Thermodynamics of Alkaline Earth Carbonates Using First-Principles Calculations”, *Surface Science*, 2022 (726) 122165
9. 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
10. 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
11. 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
  12. 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
  13. 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
  14. 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
  15. 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
  16. 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
  17. 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
  18. 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
  19. 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
  20. 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
  21. 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
  22. 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

23. 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
24. J. L. Bjorklund, J. W. Bennett, T. Z. Forbes and S. E. Mason, "Modeling of  $MAI_{12}$  Keggin Heteroatom Reactivity by Anion Adsorption", *Crystal Growth & Design*, 2019 (19) 2820-2829
25. 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
26. 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
27. J. W. Bennett, X. Huang, Y. Fang, D. M. Cwiertny, V. H. Grassian and S. E. Mason, "Methane Dissociation on  $\alpha\text{-Fe}_2\text{O}_3(0001)$  and  $\text{Fe}_3\text{O}_4(111)$  Surfaces: First-Principles Insights into Chemical Looping Combustion", *J. Phys. Chem. C.*, 2019 (123) 6450-6463
28. 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
29. 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
30. 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  $\text{Li}(\text{Ni}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3})\text{O}_2$ ", *Environ. Sci. Technol.*, 2018 (52) 5792-5802
31. 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
32. 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
33. 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  $\text{LiCoO}_2$  in a Water Environment and Implications for Reactivity under Ambient Conditions", *J. Phys. Chem. C.*, 2017 (121) 5069-5080
34. B. Monserrat, J. W. Bennett, K. M. Rabe, and D. Vanderbilt, "Antiferroelectric topological insulators in ABC compounds", *Phys. Rev. Lett.*, 2017 (119) 036802
35. 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

36. 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
37. K. F. Garrity, J. W. Bennett, K. M. Rabe and D. Vanderbilt, "Pseudopotentials for high-throughput DFT calculations", *Comp. Mater. Sci.*, 2014, (81), 446
38. J. Brehm, J. W. Bennett, M. R. Schoenberg, I. Grinberg, and A. M. Rappe, "The structural diversity of  $AB_2S_3$  compounds with  $d^0$  electronic configuration for the  $B$ -cation", *J. Chem. Phys.*, 2014 (140) 224703-1-8
39. 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  $PbTiO_3$ -based oxysulfides", *Phys. Rev. B.*, 2014 (89) 195202-1-8
40. J. W. Bennett, K. F. Garrity, K. M. Rabe, D. Vanderbilt, "Orthorhombic  $ABC$  semiconductors as antiferroelectrics", *Phys. Rev. Lett.*, 2013, (110), 017603
41. 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
42. J. W. Bennett, K. F. Garrity, K. M. Rabe and D. Vanderbilt, "Hexagonal  $ABC$  semiconductors as ferroelectrics", *Phys. Rev. Lett.*, 2012, (109) 167602
43. A. Roy, J. W. Bennett, K. M. Rabe and D. Vanderbilt, "Half-Heusler semiconductors as piezoelectrics", *Phys. Rev. Lett.* 2012, (109) 037602
44. 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  $ABB'O_3$  perovskite solid solutions", *Phys. Rev. B.*, 2011, (84), 245206
45. 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
46. J. W. Bennett, I. Grinberg, P. K. Davies and A. M. Rappe, "Pb-free ferroelectrics investigated with density-functional theory:  $Sn(Al_{1/2}Nb_{1/2})O_3$  perovskites", *Phys. Rev. B.*, 2011, (83) 144122-1-6
47. J. W. Bennett, I. Grinberg, P. K. Davies and A. M. Rappe, "Pb-free semiconductor ferroelectrics: A theoretical study of Pd-substituted  $Ba(Ti_{1-x}Ce_x)O_3$  solid solutions", *Phys. Rev. B*, 2010, (82) 184106-1-5
48. J. W. Bennett, I. Grinberg and A. M. Rappe, "The effect of substituting S for O: The sulfide perovskite  $BaZrS_3$ ", *Phys. Rev. B.*, 2009, (79) 235115-1-6
49. J. W. Bennett, I. Grinberg and A. M. Rappe, "New highly polar semi-conductor ferroelectrics through  $d^8$ -cation O-vacancy doping of  $PbTiO_3$ ", *J. Amer. Chem. Soc.*, 2008, (130), 17409-17412
50. J. W. Bennett, I. Grinberg and A. M. Rappe, "Non-monotonic composition dependence of the dielectric response of  $Ba_{1-x}Ca_xZrO_3$ ", *Chem. Mater.*, 2008, (20), 5134-5138
51. 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, " $BaCe_{1-x}Pd_xO_3$  : Redox controlled ingress and egress of palladium in a perovskite", *Chem. Mater.*, 2007, (19), 1418-1426
52. 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

53. J. W. Bennett, I. Grinberg and A.M. Rappe, "Effect of symmetry-lowering on the dielectric response of BaZrO<sub>3</sub>", *Phys. Rev. B.*, 2006, (73), 180102(R)
54. 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, "The Discovery and Design of New Materials as Multifunctional Platforms", Virginia Tech Department of Chemistry, Blacksburg, VA, October 2023
2. J. W. Bennett, "The Discovery and Design of New Materials as Multifunctional Platforms", Coppin State University, Baltimore, MD, May 2023
3. J. W. Bennett, "The Discovery and Design of New Materials as Multifunctional Platforms", University of Maryland College Park MSE, College Park, MD, May 2023
4. J. W. Bennett, "Density Functional Theory (DFT) as a Noninvasive Probe in the Field of Art Conservation Science", Millersville University, Millersville PA, September 2022
5. J. W. Bennett, "Density Functional Theory (DFT) as a Noninvasive Probe in the Field of Art Conservation Science", Lehigh Valley ACS Meeting, April 2022
6. J. W. Bennett, "Search for New Piezoelectrics, Ferroelectrics, and Antiferroelectrics", UMBC Department of Physics Colloquium, Baltimore, MD, December 2020
7. J. W. Bennett, "Atomistic Insights into Safer Water and Cleaner Energy", UMBC Department of Chemistry and Biochemistry, Baltimore, MD, November 2020
8. J. W. Bennett, "Thermodynamics of Complex Metal Oxide Surface Transformations", UMBC Department of Chemistry and Biochemistry, Baltimore, MD, USA, January 2019
9. J. W. Bennett, "DFT Methods for Modeling Nanomaterials", Tuskegee University Department of Chemistry, Tuskegee, AL, USA, September 2017



10. 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
11. J. W. Bennett, "The Search for New Functional Semiconductors", Naval Research Laboratory Electronics Science and Technology Division, Washington, D.C., USA, October 2015
12. J. W. Bennett, "Discovery and Design of Multifunctional Materials", Laboratory for Surface Modification Seminar, Rutgers University, Piscataway, NJ, USA, April 2012
13. J. W. Bennett, "Discovery and Design of Multifunctional Materials", Argonne National Lab Materials Science Division, Argonne, IL, USA March 2012
14. 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)**

15. 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
16. J. W. Bennett, "Designing New Functional Semiconductors from First-Principles", Materials Research Society Spring Meeting, online, April 2021
17. (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
18. (J. W. Bennett), K. M. Rabe\*, "New Ferroelectrics and Antiferroelectrics by Design", 7<sup>th</sup> International Conference on Electroceramics, Penn State University, State College, PA, USA, May 2015
19. 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
20. J. W. Bennett, "New Classes of Piezoelectrics, Ferroelectrics, and Antiferroelectrics by First-Principles High-Throughput Materials Design", 16<sup>th</sup> Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, Abdus Salam International Center for Theoretical Physics, Trieste, Italy, January 2013
21. J. W. Bennett, "Integration of Database Mining and First-Principles Calculations: Discovery and Design of Multifunctional Materials", 24<sup>th</sup> Annual Electronic Structure Workshop, Wake Forest University, Winston-Salem, NC, USA, June 2012
22. 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. (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
2. (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
3. (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

4. J. W. Bennett, "Design and Discovery of Solid State Ferroelectrics and Antiferroelectrics", American Chemical Society Fall Meeting, San Francisco, CA, August 2023
5. 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
6. (A. Casale), J. W. Bennett\*, "Designed Multiferroics in the  $A_2BX_3$  Family of Materials", American Chemical Society Spring Meeting, held online, April 2023
7. (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
8. (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
9. (L. Kidd), G. Trobare, A. Tauraso, J. W. Bennett\*, "A Noninvasive Computational Investigation of the Photodegradation of Vermillion", ABRCMS Anaheim, CA, November 2022
10. (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
11. 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
12. 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
13. J. W. Bennett, "The Rational Design of New Antiferroelectrics and Ferroelectrics", Materials Research Society, held online, May 2022
14. (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
15. (A. Casale), J. W. Bennett\*, "Data-Enabled Search Methods to Design New Polar Metals", American Chemical Society Spring Meeting, held online, March 2022
16. (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
17. (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
18. (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
19. J. W. Bennett, "Designing New Functional Semiconductors from First Principles", American Chemical Society Spring Meeting, held online, April 2021
20. (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

21. (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
22. (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
23. (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
24. (R. T. Grimes), J. W. Bennett\*, “First-principles Modeling of Lead Dissolution Thermodynamics in  $\text{PbCO}_3$ ”, American Chemical Society Spring Meeting, held online, April 2021
25. (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
26. (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
27. (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
28. J. W. Bennett, “Combining Database Mining and DFT to Create New Materials”, American Chemical Society Meeting, Philadelphia, PA, USA, March 2020 (\*posted online)
29. (J. W. Bennett), S. E. Mason\*, “Thermodynamics of Cation Dissolution from Complex Metal Oxides”, American Chemical Society Meeting, New Orleans, LA, USA, March 2018
30. J. W. Bennett, “Polar Compounds with Desirable Properties: Identifying New Functional Materials”, American Chemical Society Meeting, Philadelphia, PA, USA, August 2016
31. (J. W. Bennett), K. M. Rabe\*, “Semiconductive Hexagonal ABC as Ferroelectrics”, Materials Research Society Spring Meeting, San Francisco, CA, USA, April 2012
32. (J. W. Bennett), K. M. Rabe\*, “The Search for Multifunctional Polar Materials”, American Physical Society Meeting, Dallas, TX, USA, March 2011
33. (J. W. Bennett), K. M. Rabe\*, “The Search for Multifunctional Polar Materials”, Ferroelectrics Workshop, Gaithersburg, MD, USA February 2011
34. (J. W. Bennett), K. M. Rabe\*, “The Search for Multifunctional Polar Materials”, Materials Research Society Fall Meeting, Boston, MA, USA, November 2010
35. (J. W. Bennett), A. M. Rappe\*, “New Highly Polar Semiconductor Ferroelectrics for Solar Conversion”, American Physical Society Meeting, Pittsburgh, PA, USA, March 2009
36. (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
37. (J. W. Bennett), A. M. Rappe\*, “First-Principles Modeling of  $\text{BaCeO}_3$ : Stabilization of

- O-vacancies”, American Physical Society Meeting, New Orleans, LA, USA, March 2008
38. (J. W. Bennett), A. M. Rappe\*, “DFT Models as a Way to Study Pd-doped BaCeO<sub>3</sub>”, Ferroelectrics Workshop, Williamsburg, VA, USA, February 2007
  39. (J. W. Bennett), A. M. Rappe\*, “A First-Principles Approach to Modeling (Ba,Ca)ZrO<sub>3</sub>”, American Physical Society Meeting, Baltimore, MD, USA, March 2006

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

40. (A. Khan), J. W. Bennett\*, “Computational Discovery of New Functional Materials for Energy Generation and Storage, LSAMP 2021, College Park MD, USA, December 2021
41. (J. W. Bennett), S. E. Mason\*, “Thermodynamics of Complex Metal Oxide Transformations”, Midwest Theoretical Chemistry Conference”, University of Chicago, Chicago, IL, USA, June 2018
42. (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. (R. Smith), J. W. Bennett\*, “Data-Enabled Computational Chemistry to Better Understand Water Quality”, UMBC SURF, August 2023
2. (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
3. (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
4. (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
5. (J. Birenzvige), J. W. Bennett\*, “Phosphochalcogenides as Tunable Ferroelectrics”, UMBC URCAD, Baltimore, MD, April 2023
6. (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
7. (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
8. (A. Casale), J. W. Bennett\*, “Multiferroic Structures in the A<sub>2</sub>BX<sub>3</sub> Family of Materials” UMBC Chemistry & Biochemistry Graduate Research Day, Baltimore, MD, April 2023
9. (M. Layegh), J. W. Bennett\*, “Unveiling Novel 2D Materials: DFT and Thermodynamics Analysis” UMBC Chemistry & Biochemistry Graduate Research Day, Baltimore, MD, April 2023

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 2023
11. (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
12. (A. Khan), J. W. Bennett\*, “Computational Discovery of New Functional Materials for Energy Generation and Storage”, UMBC URCAD, April 2022, online
13. (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
14. (A. Casale) J. W. Bennett\*, “Data-Enabled Search Methods to Design New Polar Metals” UMBC Chemistry & Biochemistry Graduate Research Day, Baltimore, MD, April 2022
15. (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.
16. (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.
17. (A. S. Cook), J. W. Bennett\*, “Discovering and Characterizing New Functional Ferroelectric and Antiferroelectric Materials Using Computers”, UMBC URCAD, April 2021, online.
18. (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

- 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 5x
- 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 1<sup>st</sup> Year UMBC Chemistry Graduate Students during Summer Bridge

### *List of other PhD Students Committees served/serving on*

Lekan Ajiboye	degree expected in 2027
Aminah Amjad	degree expected in 2026
Leopoldo Posada-Escobar	degree expected in 2026
Alexander Paredes	degree expected in 2026
Mark Gabriana	degree expected in 2025
Shreyasi Sengupta	degree expected in 2025

Chanda Lowrance degree expected in 2023  
 Alex Sestok degree awarded in 2022

### **University activities**

- April 2023 Served as a Judge for the 3 Minute Thesis Competition
- Spring 2023 – present Member of the Research Computing Task Force
- September 2022 Retriever Recruitment
- Fall 2020 - present 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)

#### *Manuscript Reviewer for:*

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

I certify that this document is accurate and true.

Joseph W. Bennett



August 22, 2023