Joseph W Bennett

List of Publications by Year
in descending order

42 papers	2,461 citations	304368 22 h-index	329751 37 g-index
42 all docs	42 docs citations	42 times ranked	3607 citing authors

#	Article	IF	Citations
1	Developing new antiferroelectric and ferroelectric oxides and chalcogenides within the A2BX3 family. Journal of Materials Research, 2022, 37, 346-359.	1.2	2
2	Density Functional Theory (DFT) as a Nondestructive Probe in the Field of Art Conservation: Small-Molecule Adsorption on Aragonite Surfaces. ACS Applied Materials & Interfaces, 2022, 14, 13858-13871.	4.0	1
3	A Density Functional Theory (DFT) Investigation of Sulfur-Based Adsorbate Interactions on Alumina and Calcite Surfaces. Clays and Clay Minerals, 2022, 70, 370-385.	0.6	4
4	Surface Transformations of Lead Oxides and Carbonates Using First-Principles and Thermodynamics Calculations. Inorganic Chemistry, 2021, 60, 1228-1240.	1.9	10
5	Density functional theory and thermodynamics analysis of MAl12 Keggin substitution reactions: Insights into ion incorporation and experimental confirmation. Journal of Chemical Physics, 2021, 154, 064303.	1.2	7
6	A density functional theory (DFT) investigation of how small molecules and atmospheric pollutants relevant to art conservation adsorb on kaolinite. Applied Clay Science, 2021, 206, 106075.	2.6	11
7	Surveying polar materials in the Inorganic Crystal Structure Database to identify emerging structure types. Journal of Solid State Chemistry, 2020, 281, 121045.	1.4	5
8	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. Environmental Science: Nano, 2020, 7, 571-587.	2.2	18
9	Exploring the A₂BX₃ Family for New Functional Materials Using Crystallographic Database Mining and First-Principles Calculations. Journal of Physical Chemistry C, 2020, 124, 19413-19425.	1.5	2
10	Emerging investigator series: first-principles and thermodynamics comparison of compositionally-tuned delafossites: cation release from the (001) surface of complex metal oxides. Environmental Science: Nano, 2020, 7, 1642-1651.	2.2	11
11	DFT and thermodynamics calculations of surface cation release in LiCoO2. Applied Surface Science, 2020, 515, 145865.	3.1	34
12	Modeling of MAl₁₂ Keggin Heteroatom Reactivity by Anion Adsorption. Crystal Growth and Design, 2019, 19, 2820-2829.	1.4	10
13	DFT Computed Dielectric Response and THz Spectra of Organic Co-Crystals and Their Constituent Components. Molecules, 2019, 24, 959.	1.7	2
14	Methane Dissociation on Î±-Fe₂O₃(0001) and Fe₃O₄(111) Surfaces: First-Principles Insights into Chemical Looping Combustion. Journal of Physical Chemistry C, 2019, 123, 6450-6463.	1.5	23
15	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. Environmental Science & Technology, 2018, 52, 5792-5802.	4.6	57
16	First-Principles and Thermodynamics Study of Compositionally Tuned Complex Metal Oxides: Cation Release from the (001) Surface of Mn-Rich Lithium Nickel Manganese Cobalt Oxide. Inorganic Chemistry, 2018, 57, 13300-13311.	1.9	33
17	Impact of Phosphate Adsorption on Complex Cobalt Oxide Nanoparticle Dispersibility in Aqueous Media. Environmental Science & Technology, 2018, 52, 10186-10195.	4.6	27
18	Ab Initio Atomistic Thermodynamics Study of the (001) Surface of LiCoO₂ in a Water Environment and Implications for Reactivity under Ambient Conditions. Journal of Physical Chemistry C, 2017, 121, 5069-5080.	1.5	37

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19	Influence of nickel manganese cobalt oxide nanoparticle composition on toxicity toward Shewanella oneidensis MR-1: redesigning for reduced biological impact. Environmental Science: Nano, 2017, 4, 636-646.	2.2	27
20	Research highlights: comparing the biological response of nanoparticle solid solutions. Environmental Science: Nano, 2017, 4, 1428-1432.	2.2	2
21	Systematic Study of Aluminum Nanoclusters and Anion Adsorbates. Inorganic Chemistry, 2017, 56, 13014-13028.	1.9	18
22	Antiferroelectric Topological Insulators in Orthorhombic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>A</mml:mi><mml:mi>MgBi</mml:mi></mml:mrow></mml:math> Compounds (<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML") Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 612 Td (display=	2.9	30
23	The structural diversity of ABS3 compounds with d electronic configuration for the B-cation. Journal of Chemical Physics, 2014, 140, 224703.	1.2	55
24	Density functional theory study of hypothetical<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>PbTiO</mml:mtext><mml:mn>3</mml:mn> oxysulfides. Physical Review B, 2014, 89, .	1.1	30
25	Pseudopotentials for high-throughput DFT calculations. Computational Materials Science, 2014, 81, 446-452.	1.4	1,114
26	Orthorhombic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>A</mml:mi><mml:mi>B</mml:mi><mml:mi>C</mml:mi></mml:math>Semiconductors as Antiferroelectrics. Physical Review Letters, 2013, 110, 017603.	2.9	59
27	Integration of first-principles methods and crystallographic database searches for new ferroelectrics: Strategies and explorations. Journal of Solid State Chemistry, 2012, 195, 21-31.	1.4	42
28	Discovery and Design of Functional Materials: Integration of Database Searching and First Principles Calculations. Physics Procedia, 2012, 34, 14-23.	1.2	25
29	Hexagonal<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>A</mml:mi><mml:mi>B</mml:mi><mml:mi>C</mml:mi></mml:math>Semiconductors as Ferroelectrics. Physical Review Letters, 2012, 109, 167602.	2.9	114
30	Half-Heusler Semiconductors as Piezoelectrics. Physical Review Letters, 2012, 109, 037602.	2.9	180
31	Pb-free ferroelectrics investigated with density functional theory: SnAl<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>/</mml:mo><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow>	1.1	19
32	First-principles study of band gap engineering via oxygen vacancy doping in perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>A</mml:mi><mml:mi>B</mml:mi><mml:msup><mml:mi>B</mml:mi><mml:mo>â€² /</mml:mo> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>solid solutions. Physical Review B, 2011, 84, .	1.1	25
33	Studies of Perovskite Materials for High-Performance Storage Media, Piezoelectric, and Solar Energy Conversion Devices. , 2010, , .		3
34	Pb-free semiconductor ferroelectrics: A theoretical study of Pd-substituted<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Ba</mml:mtext><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:msub> Physical Review B, 2010, 82, .	1.1	48
35	Effect of substituting of S for O: The sulfide perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>BaZrS</mml:mtext></mml:mrow><mml:mn>3</mml:mn> with density functional theory. Physical Review B, 2009, 79, .	1.1	74
36	New Prospects for High Performance SONAR, Chemical Sensor, and Communication Device Materials. , 2009, , .		3

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37	New Highly Polar Semiconductor Ferroelectrics throughd⁸Cation-O Vacancy Substitution into PbTiO₃: A Theoretical Study. Journal of the American Chemical Society, 2008, 130, 17409-17412.	6.6	167
38	Modeling of Materials for Naval SONAR, Pollution Control and Nonvolatile Memory Application. , 2008, , .		0
39	BaCe1-xPdxO3-Î´(0 â‰¤xâ‰¤ 0.1):Â Redox Controlled Ingress and Egress of Palladium in a Perovskite. Chemistry of Materials, 2007, 19, 1418-1426.	3.2	46
40	Effect of symmetry lowering on the dielectric response ofBaZrO3. Physical Review B, 2006, 73, .	1.1	80
41	Baltimore SCIART: A Fully Virtual Undergraduate Research Experience at the Interface of Computational Chemistry and Art. Journal of Chemical Education, 0, , .	1.1	1
42	Examining the Aufbau Principle and Ionization Energies: A Computational Chemistry Exercise for the Introductory Level. Journal of Chemical Education, 0, , .	1.1	5