Nicole A Benedek

List of Publications by Year
in descending order

45 papers	3,179 citations	236612 25 h-index	243296 44 g-index
48 all docs	48 docs citations	48 times ranked	4191 citing authors

#	Article	IF	Citations
1	A strategy to identify materials exhibiting a large nonlinear phononics response: tuning the ultrafast structural response of LaAlO₃ with pressure. Journal of Physics Condensed Matter, 2022, 34, 035402.	0.7	3
2	Hybrid Improper Ferroelectricity: A Theoretical, Computational, and Synthetic Perspective. Annual Review of Materials Research, 2022, 52, 331-355.	4.3	9
3	Ultrafast Control of Material Optical Properties via the Infrared Resonant Raman Effect. Physical Review X, 2021, 11, .	2.8	7
4	Spin-phonon interaction in yttrium iron garnet. Physical Review B, 2021, 104, .	1.1	1
5	The influence of the 6s2 configuration of Bi3+ on the structures of Aâ€²BiNb2O7 (Aâ€² = Rb, Na, Li) layered perovskite oxides. Dalton Transactions, 2021, 50, 15359-15369.	1.6	3
6	Understanding mechanisms of thermal expansion in complex oxide thin-films from first principles: Role of high-order phonon-strain anharmonicity. Journal of Applied Physics, 2021, 130, 205106.	1.1	1
7	Polar Structures of KNdNb₂O₇ and KNdTa₂O₇. Chemistry of Materials, 2020, 32, 7965-7972.	3.2	8
8	Complex Structural Phase Transitions of the Hybrid Improper Polar Dionâ€“Jacobson Oxides RbNdM₂O₇ and CsNdM₂O₇ (M = Nb, Ta). Chemistry of Materials, 2020, 32, 4340-4346.	3.2	21
9	Strain game revisited for complex oxide thin films: Substrate-film thermal expansion mismatch in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>PbTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><m Physical Review Materials, 2020, 4, .	2.9	5
10	Thermal expansion in insulating solids from first principles. Journal of Applied Physics, 2019, 126, .	1.1	31
11	Ritz and Benedek Reply:. Physical Review Letters, 2019, 123, 179602.	2.9	1
12	Ultrafast optically induced ferromagnetic/anti-ferromagnetic phase transition in GdTiO3 from first principles. Npj Quantum Materials, 2018, 3, .	1.8	30
13	Interplay between Phonons and Anisotropic Elasticity Drives Negative Thermal Expansion in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>PbTiO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn Physical Review Letters, 2018, 121, 255901.	2.9	26
14	Cation Exchange as a Mechanism To Engineer Polarity in Layered Perovskites. Chemistry of Materials, 2018, 30, 8915-8924.	3.2	25
15	Theory and Neutrons Combine To Reveal a Family of Layered Perovskites without Inversion Symmetry. Chemistry of Materials, 2017, 29, 9489-9497.	3.2	36
16	Emergent Noncentrosymmetry and Piezoelectricity Driven by Oxygen Octahedral Rotations in n = 2 Dionâ€“Jacobson Phase Layer Perovskites. Advanced Functional Materials, 2016, 26, 1930-1937.	7.8	33
17	La₂SrCr₂O₇: Controlling the Tilting Distortions of n = 2 Ruddlesdenâ€“Popper Phases through A-Site Cation Order. Inorganic Chemistry, 2016, 55, 8951-8960.	1.9	21
18	Symmetry-Adapted Distortion Modes as Descriptors for Materials Informatics. Springer Series in Materials Science, 2016, , 213-222.	0.4	3

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19	â€˜Ferroelectricâ€™ metals reexamined: fundamental mechanisms and design considerations for new materials. Journal of Materials Chemistry C, 2016, 4, 4000-4015.	2.7	119
20	Understanding ferroelectricity in layered perovskites: new ideas and insights from theory and experiments. Dalton Transactions, 2015, 44, 10543-10558.	1.6	218
21	Enhancement of Ionic Transport in Complex Oxides through Soft Lattice Modes and Epitaxial Strain. Chemistry of Materials, 2015, 27, 2647-2652.	3.2	61
22	Interplay of Octahedral Rotations and Lone Pair Ferroelectricity in CsPbF₃. Inorganic Chemistry, 2015, 54, 8536-8543.	1.9	54
23	Origin of Ferroelectricity in a Family of Polar Oxides: The Dionâ€”Jacobson Phases. Inorganic Chemistry, 2014, 53, 3769-3777.	1.9	80
24	Polarization that Holds Steady. Physics Magazine, 2014, 7, .	0.1	8
25	Mechanical Control of Electroresistive Switching. Nano Letters, 2013, 13, 4068-4074.	4.5	55
26	Exploiting dimensionality and defect mitigation to create tunable microwave dielectrics. Nature, 2013, 502, 532-536.	13.7	204
27	Crystal-Chemical Guide for Understanding Redox Energy Variations of M^{2+/3+} Couples in Polyanion Cathodes for Lithium-Ion Batteries. Chemistry of Materials, 2013, 25, 4010-4016.	3.2	104
28	Turning ABO₃ Antiferroelectrics into Ferroelectrics: Design Rules for Practical Rotationâ€Driven Ferroelectricity in Double Perovskites and A₃B₂O₇ Ruddlesdenâ€Popper Compounds. Advanced Functional Materials, 2013, 23, 4810-4820.	7.8	187
29	Why Are There So Few Perovskite Ferroelectrics?. Journal of Physical Chemistry C, 2013, 117, 13339-13349.	1.5	373
30	Publisherâ€™s Note: Interface Control of Emergent Ferroic Order in Ruddlesden-PopperSrn+1TinO3n+1 [Phys. Rev. Lett.107, 257602 (2011).]. Physical Review Letters, 2012, 108, .	2.9	2
31	Polar octahedral rotations: A path to new multifunctional materials. Journal of Solid State Chemistry, 2012, 195, 11-20.	1.4	206
32	The magnetoelectric effect in transition metal oxides: Insights and the rational design of new materials from first principles. Current Opinion in Solid State and Materials Science, 2012, 16, 227-242.	5.6	64
33	Grain boundary stoichiometry and interactions with defects in SrTiO3. Scripta Materialia, 2012, 66, 105-108.	2.6	25
34	Hybrid Improper Ferroelectricity: A Mechanism for Controllable Polarization-Magnetization Coupling. Physical Review Letters, 2011, 106, 107204.	2.9	604
35	Interface Control of Emergent Ferroic Order in Ruddlesden-Popper<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Sr</mml:mi><mml:mrow><mml:mi>n</mml:mi><mml:mo>+</mml:mo><mml:mn>1</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mrow><mml:mn>3</mml:mn><mml:mi>n</mml:mi><mml:mo>+</mml:mo><mml:mn>1</mml:mn></mml:mrow></mml:msub></mml:math> Physical Review Letters, 2011, 107, 257602.	2.9	210
36	A genetic algorithm for predicting the structures of interfaces in multicomponent systems. Nature Materials, 2010, 9, 418-422.	13.3	152

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37	The Structure of Grain Boundaries in Strontium Titanate: Theory, Simulation, and Electron Microscopy. Annual Review of Materials Research, 2010, 40, 557-599.	4.3	47
38	Atomic-scale characterization of theSrTiO3Î£3(112)[1Â¯10]grain boundary. Physical Review B, 2010, 81, .	1.1	18
39	Interatomic potentials for strontium titanate: An assessment of their transferability and comparison with density functional theory. Physical Review B, 2008, 78, .	1.1	70
40	First principles investigation of polarisation at interfaces in multilayered strontium titanate. Journal of Physics: Conference Series, 2008, 94, 012005.	0.3	6
41	Density Functional Theory Study of Hydrogen Bonding in Ionic Molecular Materials. Journal of Physical Chemistry B, 2006, 110, 19605-19610.	1.2	6
42	Quantum Monte Carlo calculations of the dissociation energy of the water dimer. Journal of Chemical Physics, 2006, 125, 104302.	1.2	46
43	Application of numerical basis sets to hydrogen bonded systems: A density functional theory study. Journal of Chemical Physics, 2005, 122, 144102.	1.2	122
44	Quantum Monte Carlo Study of Water Molecule: A Preliminary Investigation. Australian Journal of Chemistry, 2004, 57, 1229.	0.5	3
45	Hydrogen bonding in mixed ligand copper organophosphonates. Chemical Physics Letters, 2003, 378, 400-405.	1.2	4