

# Nicole A Benedek

## List of Publications by Year in descending order

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45  
papers

3,179  
citations

236612

25  
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48  
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docs citations

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times ranked

4191  
citing authors

#	ARTICLE	IF	CITATIONS
1	Hybrid Improper Ferroelectricity: A Mechanism for Controllable Polarization-Magnetization Coupling. <i>Physical Review Letters</i> , 2011, 106, 107204.	2.9	604
2	Why Are There So Few Perovskite Ferroelectrics?. <i>Journal of Physical Chemistry C</i> , 2013, 117, 13339-13349.	1.5	373
3	Understanding ferroelectricity in layered perovskites: new ideas and insights from theory and experiments. <i>Dalton Transactions</i> , 2015, 44, 10543-10558.	1.6	218
4	Polar octahedral rotations: A path to new multifunctional materials. <i>Journal of Solid State Chemistry</i> , 2012, 195, 11-20.	1.4	206
5	Exploiting dimensionality and defect mitigation to create tunable microwave dielectrics. <i>Nature</i> , 2013, 502, 532-536.	13.7	204
6	Turning $ABO_3$ Antiferroelectrics into Ferroelectrics: Design Rules for Practical Rotation-Driven Ferroelectricity in Double Perovskites and $A_3B_2O_7$ Ruddlesden-Popper Compounds. <i>Advanced Functional Materials</i> , 2013, 23, 4810-4820.	7.8	187
7	A genetic algorithm for predicting the structures of interfaces in multicomponent systems. <i>Nature Materials</i> , 2010, 9, 418-422.	13.3	152
8	Application of numerical basis sets to hydrogen bonded systems: A density functional theory study. <i>Journal of Chemical Physics</i> , 2005, 122, 144102.	1.2	122
9	"Ferroelectric" metals reexamined: fundamental mechanisms and design considerations for new materials. <i>Journal of Materials Chemistry C</i> , 2016, 4, 4000-4015.	2.7	119
10	Crystal-Chemical Guide for Understanding Redox Energy Variations of $M^{2+/3+}$ Couples in Polyanion Cathodes for Lithium-Ion Batteries. <i>Chemistry of Materials</i> , 2013, 25, 4010-4016.	3.2	104
11	Origin of Ferroelectricity in a Family of Polar Oxides: The Dion-Jacobson Phases. <i>Inorganic Chemistry</i> , 2014, 53, 3769-3777.	1.9	80
12	Interface Control of Emergent Ferroic Order in Ruddlesden-Popper $A_nB_{n+1}O_{3n+1}$ Compounds. <i>Physical Review Letters</i> , 2011, 107, 257602.	7.8	187
13	Interatomic potentials for strontium titanate: An assessment of their transferability and comparison with density functional theory. <i>Physical Review B</i> , 2008, 78, .	1.1	70
14	The magnetoelectric effect in transition metal oxides: Insights and the rational design of new materials from first principles. <i>Current Opinion in Solid State and Materials Science</i> , 2012, 16, 227-242.	5.6	64
15	Enhancement of Ionic Transport in Complex Oxides through Soft Lattice Modes and Epitaxial Strain. <i>Chemistry of Materials</i> , 2015, 27, 2647-2652.	3.2	61
16	Mechanical Control of Electroresistive Switching. <i>Nano Letters</i> , 2013, 13, 4068-4074.	4.5	55
17	Interplay of Octahedral Rotations and Lone Pair Ferroelectricity in $CsPbF_3$ . <i>Inorganic Chemistry</i> , 2015, 54, 8536-8543.	1.9	54
18	The Structure of Grain Boundaries in Strontium Titanate: Theory, Simulation, and Electron Microscopy. <i>Annual Review of Materials Research</i> , 2010, 40, 557-599.	4.3	47

#	ARTICLE	IF	CITATIONS
19	Quantum Monte Carlo calculations of the dissociation energy of the water dimer. Journal of Chemical Physics, 2006, 125, 104302.	1.2	46
20	Theory and Neutrons Combine To Reveal a Family of Layered Perovskites without Inversion Symmetry. Chemistry of Materials, 2017, 29, 9489-9497.	3.2	36
21	Emergent Noncentrosymmetry and Piezoelectricity Driven by Oxygen Octahedral Rotations in $A_{2-2x}B_xC_{2-2x}O_{7-2x}$ Dionâ€“Jacobson Phase Layer Perovskites. Advanced Functional Materials, 2016, 26, 1930-1937.	7.8	33
22	Thermal expansion in insulating solids from first principles. Journal of Applied Physics, 2019, 126, .	1.1	31
23	Ultrafast optically induced ferromagnetic/anti-ferromagnetic phase transition in GdTiO <sub>3</sub> from first principles. Npj Quantum Materials, 2018, 3, .	1.8	30
24	Interplay between Phonons and Anisotropic Elasticity Drives Negative Thermal Expansion in $PbTiO_3$ . Physical Review Letters, 2018, 121, 255901.	2.9	26
25	Grain boundary stoichiometry and interactions with defects in SrTiO <sub>3</sub> . Scripta Materialia, 2012, 66, 105-108.	2.6	25
26	Cation Exchange as a Mechanism To Engineer Polarity in Layered Perovskites. Chemistry of Materials, 2018, 30, 8915-8924.	3.2	25
27	$La_{2-x}Sr_{x-2}Cr_2O_7$ : Controlling the Tilting Distortions of $A_{2-2x}B_xC_{2-2x}O_{7-2x}$ Ruddlesdenâ€“Popper Phases through A-Site Cation Order. Inorganic Chemistry, 2016, 55, 8951-8960.	1.9	21
28	Complex Structural Phase Transitions of the Hybrid Improper Polar Dionâ€“Jacobson Oxides $RbNdM_2O_7$ and $CsNdM_2O_7$ (M = Nb, Ta). Chemistry of Materials, 2020, 32, 4340-4346.	3.2	21
29	Atomic-scale characterization of the SrTiO <sub>3</sub> (112)[1 $\bar{1}$ 0] grain boundary. Physical Review B, 2010, 81, .	1.1	18
30	Hybrid Improper Ferroelectricity: A Theoretical, Computational, and Synthetic Perspective. Annual Review of Materials Research, 2022, 52, 331-355.	4.3	9
31	Polarization that Holds Steady. Physics Magazine, 2014, 7, .	0.1	8
32	Polar Structures of $KNdNb_2O_7$ and $KNdT_a_2O_7$ . Chemistry of Materials, 2020, 32, 7965-7972.	3.2	8
33	Ultrafast Control of Material Optical Properties via the Infrared Resonant Raman Effect. Physical Review X, 2021, 11, .	2.8	7
34	Density Functional Theory Study of Hydrogen Bonding in Ionic Molecular Materials. Journal of Physical Chemistry B, 2006, 110, 19605-19610.	1.2	6
35	First principles investigation of polarisation at interfaces in multilayered strontium titanate. Journal of Physics: Conference Series, 2008, 94, 012005.	0.3	6
36	Strain game revisited for complex oxide thin films: Substrate-film thermal expansion mismatch in $PbTiO_3$ . Physical Review Materials, 2020, 4, .	0.9	5

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37	Hydrogen bonding in mixed ligand copper organophosphonates. <i>Chemical Physics Letters</i> , 2003, 378, 400-405.	1.2	4
38	Symmetry-Adapted Distortion Modes as Descriptors for Materials Informatics. <i>Springer Series in Materials Science</i> , 2016, , 213-222.	0.4	3
39	Quantum Monte Carlo Study of Water Molecule: A Preliminary Investigation. <i>Australian Journal of Chemistry</i> , 2004, 57, 1229.	0.5	3
40	The influence of the 6s <sup>2</sup> configuration of Bi <sup>3+</sup> on the structures of A <sup>2+</sup> BiNb <sub>2</sub> O <sub>7</sub> (A <sup>2+</sup> = Rb, Na, Li) layered perovskite oxides. <i>Dalton Transactions</i> , 2021, 50, 15359-15369.	1.6	3
41	A strategy to identify materials exhibiting a large nonlinear phononics response: tuning the ultrafast structural response of LaAlO <sub>3</sub> with pressure. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 035402.	0.7	3
42	Publisher's Note: Interface Control of Emergent Ferroic Order in Ruddlesden-Popper Sr <sub>n+1</sub> Ti <sub>n</sub> O <sub>3n+1</sub> [Phys. Rev. Lett. 107, 257602 (2011)]. <i>Physical Review Letters</i> , 2012, 108, .	2.9	2
43	Ritz and Benedek Reply:. <i>Physical Review Letters</i> , 2019, 123, 179602.	2.9	1
44	Spin-phonon interaction in yttrium iron garnet. <i>Physical Review B</i> , 2021, 104, .	1.1	1
45	Understanding mechanisms of thermal expansion in complex oxide thin-films from first principles: Role of high-order phonon-strain anharmonicity. <i>Journal of Applied Physics</i> , 2021, 130, 205106.	1.1	1