James M Rondinelli

List of Publications by Year
in descending order

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231 papers	16,564 citations	17440 63 h-index	16183 124 g-index
247 all docs	247 docs citations	247 times ranked	15587 citing authors

#	Article	IF	Citations
1	Ruddlesdenâ€“Popper Hybrid Lead Iodide Perovskite 2D Homologous Semiconductors. Chemistry of Materials, 2016, 28, 2852-2867.	6.7	1,607
2	Interface-induced phenomena in magnetism. Reviews of Modern Physics, 2017, 89, .	45.6	672
3	K₃B₆O₁₀Cl: A New Structure Analogous to Perovskite with a Large Second Harmonic Generation Response and Deep UV Absorption Edge. Journal of the American Chemical Society, 2011, 133, 7786-7790.	13.7	617
4	Expanding frontiers in materials chemistry and physics with multiple anions. Nature Communications, 2018, 9, 772.	12.8	612
5	Designing a Deep-Ultraviolet Nonlinear Optical Material with a Large Second Harmonic Generation Response. Journal of the American Chemical Society, 2013, 135, 4215-4218.	13.7	542
6	Deep Ultraviolet Nonlinear Optical Materials. Chemistry of Materials, 2016, 28, 5238-5258.	6.7	481
7	Control of octahedral connectivity in perovskite oxide heterostructures: An emerging route to multifunctional materials discovery. MRS Bulletin, 2012, 37, 261-270.	3.5	378
8	Structure and Properties of Functional Oxide Thin Films: Insights From Electronicâ€Structure Calculations. Advanced Materials, 2011, 23, 3363-3381.	21.0	339
9	Estimating Hybridization of Transition Metal and Oxygen States in Perovskites from O K-edge X-ray Absorption Spectroscopy. Journal of Physical Chemistry C, 2014, 118, 1856-1863.	3.1	339
10	Cs₃Zn₆B₉O₂₁: A Chemically Benign Member of the KBBF Family Exhibiting the Largest Second Harmonic Generation Response. Journal of the American Chemical Society, 2014, 136, 1264-1267.	13.7	310
11	Carrier-mediated magnetoelectricity in complex oxide heterostructures. Nature Nanotechnology, 2008, 3, 46-50.	31.5	306
12	Quantifying octahedral rotations in strained perovskite oxide films. Physical Review B, 2010, 82, .	3.2	293
13	Three-Dimensionally Ordered Macroporous Li4Ti5O12:Â Effect of Wall Structure on Electrochemical Properties. Chemistry of Materials, 2006, 18, 482-489.	6.7	292
14	Octahedral Rotationâ€Induced Ferroelectricity in Cation Ordered Perovskites. Advanced Materials, 2012, 24, 1961-1968.	21.0	288
15	RbMgCO₃F: A New Beryllium-Free Deep-Ultraviolet Nonlinear Optical Material. Journal of the American Chemical Society, 2015, 137, 10504-10507.	13.7	283
16	Whither the oxide interface. Nature Materials, 2012, 11, 92-94.	27.5	268
17	Design and Synthesis of the Berylliumâ€Free Deepâ€Ultraviolet Nonlinear Optical Material Ba₃(ZnB₅O₁₀)PO₄. Advanced Materials, 2015, 27, 7380-7385.	21.0	262
18	Polar metals by geometric design. Nature, 2016, 533, 68-72.	27.8	262

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19	Pb₂Ba₃(BO₃)₃Cl: A Material with Large SHG Enhancement Activated by Pb-Chelated BO₃ Groups. Journal of the American Chemical Society, 2015, 137, 9417-9422.	13.7	255
20	Colloquium: Emergent properties in plane view: Strong correlations at oxide interfaces. Reviews of Modern Physics, 2014, 86, 1189-1202.	45.6	230
21	Understanding ferroelectricity in layered perovskites: new ideas and insights from theory and experiments. Dalton Transactions, 2015, 44, 10543-10558.	3.3	218
22	Mixed-Metal Carbonate Fluorides as Deep-Ultraviolet Nonlinear Optical Materials. Journal of the American Chemical Society, 2017, 139, 1285-1295.	13.7	195
23	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.	14.9	187
24	M₄Mg₄(P₂O₇)₃ (M = K, Rb): Structural Engineering of Pyrophosphates for Nonlinear Optical Applications. Chemistry of Materials, 2017, 29, 1845-1855.	6.7	187
25	Pb₂BO₃I: A Borate Iodide with the Largest Secondâ€Harmonic Generation (SHG) Response in the KBe₂BO₃F₂ (KBBF) Family of Nonlinear Optical (NLO) Materials. Angewandte Chemie - International Edition, 2018, 57, 6100-6103.	13.8	177
26	Heterointerface engineered electronic and magnetic phases of NdNiO3 thin films. Nature Communications, 2013, 4, 2714.	12.8	167
27	Improved Electrochemical Phase Diagrams from Theory and Experiment: The Niâ€“Water System and Its Complex Compounds. Journal of Physical Chemistry C, 2017, 121, 9782-9789.	3.1	163
28	Non-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mi>d</mml:mi><mml:mn>0</mml:mn></mml:msup></mml:mrow></mml:math>Mn-dr ferroelectricity in antiferromagnetic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BaMnO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml: Physical Review B, 2009, 79, .	3.2	162
29	Asymmetric Orbital-Lattice Interactions in Ultrathin Correlated Oxide Films. Physical Review Letters, 2011, 107, 116805.	7.8	158
30	Extreme tensile strain states in La _{0.7} Ca _{0.3} MnO ₃ membranes. Science, 2020, 368, 71-76.	12.6	151
31	Berylliumâ€Free Î²â€²Rb₂Al₂B₂O₇ as a Possible Deepâ€Ultraviolet Nonlinear Optical Material Replacement for KBe₂BO₃F₂. Angewandte Chemie - International Edition, 2017, 56, 2969-2973.	13.8	150
32	Heteroanionic Materials by Design: Progress Toward Targeted Properties. Advanced Materials, 2019, 31, e1805295.	21.0	150
33	Electronic properties of bulk and thin film<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SrRuO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml: Search for the metal-insulator transition. Physical Review B, 2008, 78, .	3.2	143
34	Bidenticity-Enhanced Second Harmonic Generation from Pb Chelation in Pb₃Mg₃TeP₂O₁₄. Journal of the American Chemical Society, 2016, 138, 88-91.	13.7	143
35	The must-have and nice-to-have experimental and computational requirements for functional frequency doubling deep-UV crystals. Nature Communications, 2018, 9, 2972.	12.8	137
36	Designing a robustly metallic noncenstrosymmetric ruthenate oxide with large thermopower anisotropy. Nature Communications, 2014, 5, 3432.	12.8	134

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37	Effect of Interfacial Octahedral Behavior in Ultrathin Manganite Films. Nano Letters, 2014, 14, 2509-2514.	9.1	121
38	Symbolic regression in materials science. MRS Communications, 2019, 9, 793-805.	1.8	119
39	Electronic, Crystal Chemistry, and Nonlinear Optical Property Relationships in the Dugganite A₃B₃CD₂O₁₄ Family. Journal of the American Chemical Society, 2016, 138, 4984-4989.	13.7	118
40	Octahedral Rotation Preferences in Perovskite Iodides and Bromides. Journal of Physical Chemistry Letters, 2016, 7, 918-922.	4.6	115
41	Theory-Guided Machine Learning in Materials Science. Frontiers in Materials, 2016, 3, .	2.4	112
42	Chemical gradients in human enamel crystallites. Nature, 2020, 583, 66-71.	27.8	112
43	Lattice normal modes and electronic properties of the correlated metal LaNiO<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>. Physical Review B, 2011, 84, .	3.2	110
44	Interplay of Octahedral Tilts and Polar Order in BiFeO₃ Films. Advanced Materials, 2013, 25, 2497-2504.	21.0	101
45	Band structure and optical transitions in LaFeO₃: theory and experiment. Journal of Physics Condensed Matter, 2014, 26, 505502.	1.8	100
46	Substrate coherency driven octahedral rotations in perovskite oxide films. Physical Review B, 2010, 82, .	3.2	95
47	Epitaxial-strain-induced polar-to-nonpolar transitions in layered oxides. Nature Materials, 2016, 15, 951-955.	27.5	94
48	Structural effects on the spin-state transition in epitaxially strained<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaCoO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2009, 79, .	3.2	89
49	Ferroelectric Sr₃Zr₂O₇: Competition between Hybrid Improper Ferroelectric and Antiferroelectric Mechanisms. Advanced Functional Materials, 2018, 28, 1801856.	14.9	89
50	Role of Acentric Displacements on the Crystal Structure and Second-Harmonic Generating Properties of RbPbCO₃F and CsPbCO₃F. Inorganic Chemistry, 2014, 53, 6241-6251.	4.0	85
51	Interplay of octahedral rotations and breathing distortions in charge-ordering perovskite oxides. Physical Review B, 2013, 88, .	3.2	77
52	Learning from data to design functional materials without inversion symmetry. Nature Communications, 2017, 8, 14282.	12.8	76
53	Microscopic Origins of Optical Second Harmonic Generation in Noncentrosymmetricâ€“Nonpolar Materials. Chemistry of Materials, 2014, 26, 5773-5781.	6.7	74
54	Hybrid Improper Ferroelectricity in (Sr,Ca)₃Sn₂O₇ and Beyond: Universal Relationship between Ferroelectric Transition Temperature and Tolerance Factor in n = 2 Ruddlesdenâ€“Popper Phases. Journal of the American Chemical Society, 2018, 140, 15690-15700.	13.7	74

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55	Crystal-Chemistry Guidelines for Noncentrosymmetric A₂BO₄ Ruddlesdenâ^'Popper Oxides. Inorganic Chemistry, 2014, 53, 336-348.	4.0	73
56	Berylliumâ€Free Î²â€Rb₂Al₂B₂O₇ as a Possible Deepâ€Ultraviolet Nonlinear Optical Material Replacement for KBe₂BO₃F₂. Angewandte Chemie, 2017, 129, 3015-3019.	2.0	72
57	Polarization screening-induced magnetic phase gradients at complex oxide interfaces. Nature Communications, 2015, 6, 6735.	12.8	71
58	Materials Prediction via Classification Learning. Scientific Reports, 2015, 5, 13285.	3.3	68
59	The Nextâ€Generation of Nonlinear Optical Materials: Rb₃Ba₃Li₂Al₄B₆O₂₀Fâ€”Synthesis, Characterization, and Crystal Growth. Advanced Optical Materials, 2017, 5, 1700840.	7.3	68
60	Crystal structure and electronic properties of bulk and thin film brownmillerite oxides. Physical Review B, 2015, 92, .	3.2	67
61	Strain-induced nonsymmorphic symmetry breaking and removal of Dirac semimetallic nodal line in an orthoperovskite iridate. Physical Review B, 2016, 93, .	3.2	67
62	Covalent dependence of octahedral rotations in orthorhombic perovskite oxides. Journal of Chemical Physics, 2014, 141, 114704.	3.0	65
63	An efficient ab-initio quasiharmonic approach for the thermodynamics of solids. Computational Materials Science, 2016, 120, 84-93.	3.0	65
64	Design of a Mott Multiferroic from a Nonmagnetic Polar Metal. Physical Review Letters, 2015, 115, 087202.	7.8	64
65	Observation of Quasi-Two-Dimensional Polar Domains and Ferroelastic Switching in a Metal, Ca₃Ru₂O₇. Nano Letters, 2018, 18, 3088-3095.	9.1	62
66	Thickness-Dependent Crossover from Charge- to Strain-Mediated Magnetoelectric Coupling in Ferromagnetic/Piezoelectric Oxide Heterostructures. ACS Nano, 2014, 8, 894-903.	14.6	61
67	Inversion Symmetry Breaking by Oxygen Octahedral Rotations in the Ruddlesden-Popper<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Na</mml:mi><mml:mi>R</mml:mi><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mr Physical Review Letters, 2014, 112, 187602.	7.8	60
68	Normal mode determination of perovskite crystal structures with octahedral rotations: theory and applications. Journal of Physics Condensed Matter, 2013, 25, 175902.	1.8	59
69	Multi-messenger nanoprobes of hidden magnetism in a strained manganite. Nature Materials, 2020, 19, 397-404.	27.5	59
70	Anharmonic lattice interactions in improper ferroelectrics for multiferroic design. Journal of Physics Condensed Matter, 2015, 27, 283202.	1.8	57
71	Predicting and Designing Optical Properties of Inorganic Materials. Annual Review of Materials Research, 2015, 45, 491-518.	9.3	56
72	Correlation effects and spin-orbit interactions in two-dimensional hexagonal 5d transition metal carbides, Ta _{n+1} C _n (n = 1,2,3). Europhysics Letters, 2013, 101, 57004.	2.0	54

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73	A-Site Ordered Double Perovskite CaMnTi₂O₆ as a Multifunctional Piezoelectric and Ferroelectricâ€“Photovoltaic Material. Inorganic Chemistry, 2017, 56, 11854-11861.	4.0	54
74	First-principles study of misfit strain-stabilized ferroelectric SnTiO<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>. Physical Review B, 2011, 84, .	3.2	49
75	Domain topology and domain switching kinetics in a hybrid improper ferroelectric. Nature Communications, 2016, 7, 11602.	12.8	46
76	Surface Reconstruction with a Fractional Hole:(5Ã—5)R26.6Â°LaAlO3(001). Physical Review Letters, 2007, 98, 086102.	7.8	45
77	Large Isosymmetric Reorientation of Oxygen Octahedra Rotation Axes in Epitaxially Strained Perovskites. Physical Review Letters, 2011, 106, 235502.	7.8	45
78	Localized Symmetry Breaking for Tuning Thermal Expansion in ScF₃ Nanoscale Frameworks. Journal of the American Chemical Society, 2018, 140, 4477-4480.	13.7	44
79	Atomic Scale Design of Polar Perovskite Oxides without Second-Order Jahnâ€“Teller Ions. Chemistry of Materials, 2013, 25, 4545-4550.	6.7	41
80	Connecting bulk symmetry and orbital polarization in strained RNiO<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>ultrathin films. Physical Review B, 2013, 88, .	3.2	40
81	Modeling Corrosion with First-Principles Electrochemical Phase Diagrams. Annual Review of Materials Research, 2019, 49, 53-77.	9.3	40
82	Spectral Addressability in a Modular Two Qubit System. Journal of the American Chemical Society, 2021, 143, 8069-8077.	13.7	39
83	Interplay of Cation Ordering and Ferroelectricity in Perovskite Tin Iodides: Designing a Polar Halide Perovskite for Photovoltaic Applications. Inorganic Chemistry, 2017, 56, 26-32.	4.0	37
84	Massive band gap variation in layered oxides through cation ordering. Nature Communications, 2015, 6, 6191.	12.8	36
85	Evidence for the weakly coupled electron mechanism in an Anderson-Blount polar metal. Nature Communications, 2019, 10, 3217.	12.8	36
86	Electrochemical phase diagrams for Ti oxides from density functional calculations. Physical Review B, 2015, 92, .	3.2	35
87	Polar Oxides without Inversion Symmetry through Vacancy and Chemical Order. Journal of the American Chemical Society, 2017, 139, 2833-2841.	13.7	34
88	Strain-controlled band engineering and self-doping in ultrathin LaNiO<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>films. Physical Review B, 2012, 85, .	3.2	33
89	Structural Diversity from Anion Order in Heteroanionic Materials. Chemistry of Materials, 2018, 30, 3528-3537.	6.7	33
90	Tunable Negative Thermal Expansion in Layered Perovskites from Quasi-Two-Dimensional Vibrations. Physical Review Letters, 2016, 117, 115901.	7.8	32

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91	Ferroelectric Oxides with Strong Visible-Light Absorption from Charge Ordering. Chemistry of Materials, 2017, 29, 2445-2451.	6.7	32
92	Tunable metal-insulator transition, Rashba effect and Weyl Fermions in a relativistic charge-ordered ferroelectric oxide. Nature Communications, 2018, 9, 492.	12.8	31
93	Nonlinear phononic control and emergent magnetism in Mott insulating titanates. Physical Review B, 2018, 98, .	3.2	31
94	Anisotropic magnetoresistance in the itinerant antiferromagnetic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>EuTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2019, 99, .	3.2	31
95	Spectral manipulation in Fabry-Perot lasers: perturbative inverse scattering approach. Journal of the Optical Society of America B: Optical Physics, 2006, 23, 1046.	2.1	30
96	Understanding Chemical Bonding in Alloys and the Representation in Atomistic Simulations. Journal of Physical Chemistry C, 2018, 122, 14996-15009.	3.1	30
97	Reliable electrochemical phase diagrams of magnetic transition metals and related compounds from high-throughput ab initio calculations. Npj Materials Degradation, 2019, 3, .	5.8	30
98	Tuning the ferroelectric polarization in AAâ€²MnWO₆ double perovskites through A cation substitution. Dalton Transactions, 2015, 44, 10644-10653.	3.3	29
99	Spin-assisted covalent bond mechanism in â€œcharge-orderingâ€•perovskite oxides. Physical Review B, 2012, 86, .	3.2	28
100	Electronic structure of negative charge transfer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CaFeO</mml:mi><mml:mn>3</mml:mn></mml:msub></r across the metal-insulator transition. Physical Review Materials, 2018, 2, .	2.4	28
101	Octahedral engineering of orbital polarizations in charge transfer oxides. Physical Review B, 2013, 87, .	3.2	27
102	Assessing exchange-correlation functional performance for structure and property predictions of oxyfluoride compounds from first principles. Physical Review B, 2016, 94, .	3.2	27
103	Design of noncentrosymmetric perovskites from centric and acentric basic building units. Journal of Materials Chemistry C, 2016, 4, 4016-4027.	5.5	27
104	Role of 2D and 3D defects on the reduction of LaNiO3 nanoparticles for catalysis. Scientific Reports, 2017, 7, 10080.	3.3	27
105	Research Update: Towards designed functionalities in oxide-based electronic materials. APL Materials, 2015, 3, .	5.1	26
106	Lithium Niobate-Type Oxides as Visible Light Photovoltaic Materials. Chemistry of Materials, 2016, 28, 25-29.	6.7	26
107	Linear and nonlinear optical probe of the ferroelectric-like phase transition in a polar metal, LiOsO3. Applied Physics Letters, 2018, 113, .	3.3	26
108	Featureless adaptive optimization accelerates functional electronic materials design. Applied Physics Reviews, 2020, 7, .	11.3	26

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109	Contributions of Correlated Acentric Atomic Displacements to the Nonlinear Second Harmonic Generation and Response. ACS Photonics, 2014, 1, 96-100.	6.6	25
110	Structure Tuning, Strong Second Harmonic Generation Response, and High Optical Stability of the Polar Semiconductors Na_{1â€“x}K_xAsQ₂. Journal of the American Chemical Society, 2021, 143, 18204-18215.	13.7	24
111	Ferroelectricity from coupled cooperative Jahn-Teller distortions and octahedral rotations in ordered Ruddlesden-Popper manganates. Physical Review B, 2015, 92, .	3.2	23
112	Polar metals as electrodes to suppress the critical-thickness limit in ferroelectric nanocapacitors. Journal of Applied Physics, 2018, 124, .	2.5	23
113	Synergistically Optimizing Carrier Concentration and Decreasing Sound Velocity in n-type AgInSe₂ Thermoelectrics. Chemistry of Materials, 2019, 31, 8182-8190.	6.7	23
114	Assessing exchange-correlation functional performance in the chalcogenide lacunar spinels <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ga</mml:mi><mml:msub><mml:mi>M</mml:mi><mml:m <mml:math		

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127	Persistent polar distortions from covalent interactions in doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub> Physical Review B, 2020, 102, .	3.2	18
128	Anion Ordered and Ferroelectric Ruddlesdenâ€“Popper Oxynitride Ca₃Nb₂N₂O₅ for Visible-Light-Active Photocatalysis. Chemistry of Materials, 2020, 32, 2815-2823.	6.7	18
129	Effect of fluoropolymer composition on topochemical synthesis of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>SrMn</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mrow><mml:mn>3</mml:mn><mml:mtext>â^’</mml:mtext><mml:mi>Î´</mml:mi></mml:mrow></mml:msub><mml:mi mathvariant="normal">F</mml:mi><mml:mi>Î´</mml:mi></mml:mrow></mml:math> oxyfluoride films. Physical Review Materials, 2018, 2, .	2.4	18
130	Discovery Principles and Materials for Symmetry-Protected Persistent Spin Textures with Long Spin Lifetimes. Matter, 2020, 3, 1211-1225.	10.0	17
131	Computationally Directed Discovery of MoBi₂. Journal of the American Chemical Society, 2021, 143, 214-222.	13.7	17
132	Ferroelectricity: Octahedral Rotationâ€Induced Ferroelectricity in Cation Ordered Perovskites (Adv.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	21.0	16
133	Electrochemical phase diagrams of Ni fromab initiosimulations: role of exchange interactions on accuracy. Journal of Physics Condensed Matter, 2017, 29, 475501.	1.8	16
134	Learning from Correlations Based on Local Structure: Rare-Earth Nickelates Revisited. Journal of Chemical Information and Modeling, 2018, 58, 2491-2501.	5.4	16
135	Giant Nonâ€Resonant Infrared Second Order Nonlinearity in Î³â€‰â€NaAsSe₂. Advanced Optical Materials, 2022, 10, .	7.3	16
136	Piezoelectricity Across a Strainâ€Induced Isosymmetric Ferriâ€toâ€Ferroelectric Transition. Advanced Materials Interfaces, 2014, 1, 1400042.	3.7	15
137	Role of orbital filling on nonlinear ionic Raman scattering in perovskite titanates. Physical Review B, 2017, 95, .	3.2	15
138	First-Principles Hydrothermal Synthesis Design to Optimize Conditions and Increase the Yield of Quaternary Heteroanionic Oxychalcogenides. Chemistry of Materials, 2021, 33, 2726-2741.	6.7	15
139	Discovery of highly polarizable semiconductors BaZrS3 and Ba3Zr2S7. Physical Review Materials, 2020, 4, .	2.4	15
140	Mismatched lattices patched up. Nature Chemistry, 2016, 8, 292-294.	13.6	14
141	Structure Dependent Phase Stability and Thermal Expansion of Ruddlesdenâ€“Popper Strontium Titanates. Chemistry of Materials, 2018, 30, 7100-7110.	6.7	14
142	Cooperative interactions govern the fermiology of the polar metal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ca</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>7</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review Research, 2020, 2, .	3.6	14
143	Reconstructive Transitions from Rotations of Rigid Heteroanionic Polyhedra. Journal of the American Chemical Society, 2016, 138, 11882-11889.	13.7	13
144	Magnetoelectric coupling in the type-I multiferroic ScFeO3. Physical Review B, 2016, 94, .	3.2	13

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145	Metals amassing transparency. Nature Materials, 2016, 15, 132-134.	27.5	13
146	Synthetic investigation of competing magnetic interactions in 2D metalâ€“chloranilate radical frameworks. Chemical Science, 2020, 11, 5922-5928.	7.4	13
147	Controlled nâ€Doping of Naphthaleneâ€Diimideâ€Based 2D Polymers. Advanced Materials, 2022, 34, e2101932.	21.0	13
148	Low Thermal Conductivity in Heteroanionic Materials with Layers of Homoleptic Polyhedra. Journal of the American Chemical Society, 2022, 144, 2569-2579.	13.7	13
149	Inductive crystal field control in layered metal oxides with correlated electrons. APL Materials, 2014, 2, .	5.1	12
150	Design of Heteroanionic MoON Exhibiting a Peierls Metal-Insulator Transition. Physical Review Letters, 2019, 123, 236402.	7.8	12
151	Uncorrelated Bi off-centering and the insulator-to-metal transition in ruthenium A2Ru2O7 pyrochlores. Physical Review Materials, 2019, 3, .	2.4	12
152	Instrumental insights. Nature Materials, 2012, 11, 833-834.	27.5	11
153	Electronically driven structural transitions inA₁₀(PO₄)₆F₂apatites (A= Ca, Sr, Pb, Cd) Tj ETQq1 1 0.784314 rgBT 2014, 70, 612-615.	1.1	11
154	Catalytic Enhancement of CO Oxidation on LaFeO₃ Regulated by Ruddlesdenâ€“Popper Stacking Faults. ACS Applied Materials & Interfaces, 2019, 11, 33850-33858.	8.0	11
155	Understanding Electrochemical Stabilities of Ni-Based Nanofilms from a Comparative Theoryâ€“Experiment Approach. Journal of Physical Chemistry C, 2019, 123, 28925-28940.	3.1	11
156	Multimodal Structure Solution with 19F NMR Crystallography of Spin Singlet Molybdenum Oxyfluorides. Journal of the American Chemical Society, 2020, 142, 12288-12298.	13.7	11
157	Comprehensive anisotropic linear optical properties of the Weyl semimetals TaAs and NbAs. Physical Review B, 2021, 103, .	3.2	11
158	Enhancing structure relaxations for first-principles codes: An approximate Hessian approach. Computational Materials Science, 2007, 40, 345-353.	3.0	10
159	Strain-Induced Anion-Site Occupancy in Perovskite Oxyfluoride Films. Chemistry of Materials, 2021, 33, 1811-1820.	6.7	10
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