

James M Rondinelli

List of Publications by Year in descending order

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papers

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17405

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docs citations

247
times ranked

15587
citing authors

#	ARTICLE	IF	CITATIONS
19	Comprehensive anisotropic linear optical properties of the Weyl semimetals TaAs and NbAs. <i>Physical Review B</i> , 2021, 103, .	1.1	11
20	Spectral Addressability in a Modular Two Qubit System. <i>Journal of the American Chemical Society</i> , 2021, 143, 8069-8077.	6.6	39
21	Tunable magnetic anisotropy in multiferroic oxides. <i>Physical Review B</i> , 2021, 103, .	1.1	3
22	Negative thermal expansion in the Ruddlesden-Popper calcium titanates. <i>Physical Review Materials</i> , 2021, 5, .	0.9	7
23	First-Principles-Based Prediction of Electrochemical Oxidation and Corrosion of Copper under Multiple Environmental Factors. <i>Journal of Physical Chemistry C</i> , 2021, 125, 14027-14038.	1.5	7
24	AB ₂ X ₆ Compounds and the Stabilization of Trirutile Oxides. <i>Inorganic Chemistry</i> , 2021, 60, 9224-9232.	1.9	3
25	Polar Ferromagnetic Metal by Intercalation of Metal–Amine Complexes. <i>Chemistry of Materials</i> , 2021, 33, 4936-4947.	3.2	8
26	Database, Features, and Machine Learning Model to Identify Thermally Driven Metal–Insulator Transition Compounds. <i>Chemistry of Materials</i> , 2021, 33, 5591-5605.	3.2	20
27	Physical insights on the low lattice thermal conductivity of AgInSe ₂ . <i>Materials Today Physics</i> , 2021, 19, 100428.	2.9	20
28	Strain-Induced Magnetic Transitions in SrMO _{2.5} (M = Mn, Fe) Thin Films with Ordered Oxygen Vacancies. <i>Inorganic Chemistry</i> , 2021, 60, 13161-13167.	1.9	1
29	Energy contour exploration with potentiostatic kinematics. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 445901.	0.7	3
30	Durable Multimetal Oxychloride Intergrowths for Visible Light-Driven Water Splitting. <i>Chemistry of Materials</i> , 2021, 33, 347-358.	3.2	19
31	Computationally Directed Discovery of MoBi ₂ . <i>Journal of the American Chemical Society</i> , 2021, 143, 214-222.	6.6	17
32	Heteroanionic Ruddlesden-Popper ferroelectrics from anion order and octahedral tilts. <i>Physical Review Materials</i> , 2021, 5, .	0.9	0
33	Structure Tuning, Strong Second Harmonic Generation Response, and High Optical Stability of the Polar Semiconductors Na _{1-x} K _x As ₂ Q ₂ . <i>Journal of the American Chemical Society</i> , 2021, 143, 18204-18215.	6.6	24
34	Strong Magnetocrystalline Anisotropy Arising from Metal–Ligand Covalency in a Metal–Organic Candidate for 2D Magnetic Order. <i>Chemistry of Materials</i> , 2021, 33, 8712-8721.	3.2	8
35	Perovskite-like K ₃ TiOF ₅ Exhibits (3 + 1)-Dimensional Commensurate Structure Induced by Octahedrally Coordinated Potassium Ions. <i>Journal of the American Chemical Society</i> , 2021, 143, 18907-18916.	6.6	4
36	Phase transitions and potential ferroelectricity in noncentrosymmetric KNaNbOF ₅ . <i>Physical Review Materials</i> , 2021, 5, .	0.9	1

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37	Cu ₄ MnGe ₂ S ₇ and Cu ₂ MnGeS ₄ : two polar thio germanates exhibiting second harmonic generation in the infrared and structures derived from hexagonal diamond. Dalton Transactions, 2021, 50, 17524-17537.	1.6	9
38	Multi-messenger nanoprobos of hidden magnetism in a strained manganite. Nature Materials, 2020, 19, 397-404.	13.3	59
39	Discovery Principles and Materials for Symmetry-Protected Persistent Spin Textures with Long Spin Lifetimes. Matter, 2020, 3, 1211-1225.	5.0	17
40	Persistent polar distortions from covalent interactions in doped BaTiO_3 . Physical Review B, 2020, 102, .	1.1	2
41	Pressure-Induced Collapse of Magnetic Order in Jarosite. Physical Review Letters, 2020, 125, 077202.	2.9	3
42	Pressure effects on magnetism in Ca_2O_5 -type ferrites and manganites. Physical Review B, 2020, 102, .	1.1	2
43	Featureless adaptive optimization accelerates functional electronic materials design. Applied Physics Reviews, 2020, 7, .	5.5	26
44	Synthetic investigation of competing magnetic interactions in 2D metal-chloranilate radical frameworks. Chemical Science, 2020, 11, 5922-5928.	3.7	13
45	Multimodal Structure Solution with ¹⁹ F NMR Crystallography of Spin Singlet Molybdenum Oxyfluorides. Journal of the American Chemical Society, 2020, 142, 12288-12298.	6.6	11
46	Exploiting Colorimetry for Fidelity in Data Visualization. Chemistry of Materials, 2020, 32, 5455-5460.	3.2	6
47	Extreme tensile strain states in La _{0.7} Ca _{0.3} MnO ₃ membranes. Science, 2020, 368, 71-76.	6.0	151
48	Anion Ordered and Ferroelectric Ruddlesden-Popper Oxynitride Ca ₃ Nb ₂ N ₂ O ₅ for Visible-Light-Active Photocatalysis. Chemistry of Materials, 2020, 32, 2815-2823.	3.2	18
49	Chemical gradients in human enamel crystallites. Nature, 2020, 583, 66-71.	13.7	112
50	Uniaxial Strain-Controlled Ground States in Manganite Films. Nano Letters, 2020, 20, 1131-1140.	4.5	21
51	Microscopic Insights into the Reconstructive Phase Transition of KNaNbOF ₅ with ¹⁹ F NMR Spectroscopy. Chemistry of Materials, 2020, 32, 5715-5722.	3.2	5
52	Ferri-chiral compounds with potentially switchable Dresselhaus spin splitting. Physical Review B, 2020, 102, .	1.1	4
53	Discovery of highly polarizable semiconductors BaZrS ₃ and Ba ₃ Zr ₂ S ₇ . Physical Review Materials, 2020, 4, .	0.9	15
54	Structural signatures of the insulator-to-metal transition in BaCo_2S_2 . Physical Review Materials, 2020, 4, .	0.9	6

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55	Cooperative interactions govern the fermiology of the polar metal CaMn_3O_7 . Physical Review Research, 2020, 2, .	1.3	14
56	Evidence for an extended critical fluctuation region above the polar ordering transition in LiOsO_3 . Physical Review Research, 2020, 2, .	1.3	5
57	Hybrid improper antiferroelectricity—New insights for novel device concepts. MRS Advances, 2020, 5, 3521-3545.	0.5	1
58	Design of New Multiferroic Oxides. , 2020, , 1151-1212.		1
59	Deliberate Deficiencies: Expanding Electronic Function through Non-stoichiometry. Matter, 2019, 1, 33-35.	5.0	8
60	Property control from polyhedral connectivity in ABO_3 oxides. Physical Review B, 2019, 100, .	1.1	7
61	Symbolic regression in materials science. MRS Communications, 2019, 9, 793-805.	0.8	119
62	Evidence for the weakly coupled electron mechanism in an Anderson-Blount polar metal. Nature Communications, 2019, 10, 3217.	5.8	36
63	Atomic and electronic structure of domains walls in a polar metal. Physical Review B, 2019, 99, .	1.1	19
64	Covalency-driven Structural Evolution in the Polar Pyrochlore Series $\text{Cd}_2\text{Nb}_2\text{O}_7$ — S_x . Chemistry of Materials, 2019, 31, 7626-7637.	3.2	18
65	Catalytic Enhancement of CO Oxidation on LaFeO_3 Regulated by Ruddlesden—Popper Stacking Faults. ACS Applied Materials & Interfaces, 2019, 11, 33850-33858.	4.0	11
66	Synergistically Optimizing Carrier Concentration and Decreasing Sound Velocity in n-type AgInSe_2 Thermoelectrics. Chemistry of Materials, 2019, 31, 8182-8190.	3.2	23
67	Predicting the Structure Stability of Layered Heteroanionic Materials Exhibiting Anion Order. Inorganic Chemistry, 2019, 58, 13229-13240.	1.9	9
68	Assessing exchange-correlation functional performance in the chalcogenide lacunar spinels GaM		

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73	MnBi ₂ : A Metastable High-Pressure Phase in the Mn-Bi System. Chemistry of Materials, 2019, 31, 3083-3088.	3.2	6
74	Modeling Corrosion with First-Principles Electrochemical Phase Diagrams. Annual Review of Materials Research, 2019, 49, 53-77.	4.3	40
75	Heteroanionic Materials by Design: Progress Toward Targeted Properties. Advanced Materials, 2019, 31, e1805295.	11.1	150
76	Ultrafast quasiparticle dynamics in the correlated semimetal Ca ₃ Ru ₂ O ₇ . Physical Review B, 2019, 99, .	1.1	8
77	Understanding Electrochemical Stabilities of Ni-Based Nanofilms from a Comparative Theory-Experiment Approach. Journal of Physical Chemistry C, 2019, 123, 28925-28940.	1.5	11
78	Design of Heteroanionic MoON Exhibiting a Peierls Metal-Insulator Transition. Physical Review Letters, 2019, 123, 236402.	2.9	12
79	Probing single-unit-cell resolved electronic structure modulations in oxide superlattices with standing-wave photoemission. Physical Review B, 2019, 100, .	1.1	3
80	Design of New Multiferroic Oxides. , 2019, , 1-62.		0
81	Anisotropic magnetoresistance in the itinerant antiferromagnetic EuTi_3O_7 . Physical Review B, 2019, 99, .	1.1	31
82	High-pressure synthesis of the $\text{BiV}_3\text{O}_{10}$ perovskite. Physical Review Materials, 2019, 3, .	0.9	7
83	A^{site} cation size effect on oxygen octahedral rotations in acentric Ruddlesden-Popper alkali rare-earth titanates. Physical Review Materials, 2019, 3, .	0.9	7
84	Uncorrelated Bi off-centering and the insulator-to-metal transition in ruthenium $\text{A}_2\text{Ru}_2\text{O}_7$ pyrochlores. Physical Review Materials, 2019, 3, .	0.9	12
85	Pb_2BO_3 : A Borate Iodide with the Largest Second-Harmonic Generation (SHG) Response in the $\text{KBe}_2\text{BO}_3\text{F}_2$ (KBBF) Family of Nonlinear Optical (NLO) Materials. Angewandte Chemie - International Edition, 2018, 57, 6100-6103.	7.2	177
86	Pb_2BO_3 : A Borate Iodide with the Largest Second-Harmonic Generation (SHG) Response in the $\text{KBe}_2\text{BO}_3\text{F}_2$ (KBBF) Family of Nonlinear Optical (NLO) Materials. Angewandte Chemie, 2018, 130, 6208-6211.	1.6	22
87	Crystal structure stability and electronic properties of the layered nickelate La_4O_{10} . Physical Review B, 2018, 97, .	1.1	8
88	Expanding frontiers in materials chemistry and physics with multiple anions. Nature Communications, 2018, 9, 772.	5.8	612
89	Observation of Quasi-Two-Dimensional Polar Domains and Ferroelastic Switching in a Metal, $\text{Ca}_3\text{Ru}_2\text{O}_7$. Nano Letters, 2018, 18, 3088-3095.	4.5	62
90	Tunable metal-insulator transition, Rashba effect and Weyl Fermions in a relativistic charge-ordered ferroelectric oxide. Nature Communications, 2018, 9, 492.	5.8	31

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91	Structural Diversity from Anion Order in Heteroanionic Materials. Chemistry of Materials, 2018, 30, 3528-3537.	3.2	33
92	Localized Symmetry Breaking for Tuning Thermal Expansion in ScF ₃ Nanoscale Frameworks. Journal of the American Chemical Society, 2018, 140, 4477-4480.	6.6	44
93	Polar metals as electrodes to suppress the critical-thickness limit in ferroelectric nanocapacitors. Journal of Applied Physics, 2018, 124, .	1.1	23
94	Structure Dependent Phase Stability and Thermal Expansion of Ruddlesden-Popper Strontium Titanates. Chemistry of Materials, 2018, 30, 7100-7110.	3.2	14
95	Linear and nonlinear optical probe of the ferroelectric-like phase transition in a polar metal, LiOsO ₃ . Applied Physics Letters, 2018, 113, .	1.5	26
96	Hybrid Improper Ferroelectricity in (Sr,Ca) ₃ Sn ₂ O ₇ and Beyond: Universal Relationship between Ferroelectric Transition Temperature and Tolerance Factor in $n = 2$ Ruddlesden-Popper Phases. Journal of the American Chemical Society, 2018, 140, 15690-15700.	6.6	74
97	Coupled Raman-Raman modes in the ionic Raman scattering process. Applied Physics Letters, 2018, 113, 112903.	1.5	1
98	Discovery of Cu ₃ Pb. Angewandte Chemie, 2018, 130, 12991-12995.	1.6	3
99	Discovery of Cu ₃ Pb. Angewandte Chemie - International Edition, 2018, 57, 12809-12813.	7.2	7
100	Learning from Correlations Based on Local Structure: Rare-Earth Nickelates Revisited. Journal of Chemical Information and Modeling, 2018, 58, 2491-2501.	2.5	16
101	Ferroelectric Sr ₃ Zr ₂ O ₇ : Competition between Hybrid Improper Ferroelectric and Antiferroelectric Mechanisms. Advanced Functional Materials, 2018, 28, 1801856.	7.8	89
102	Understanding Chemical Bonding in Alloys and the Representation in Atomistic Simulations. Journal of Physical Chemistry C, 2018, 122, 14996-15009.	1.5	30
103	The must-have and nice-to-have experimental and computational requirements for functional frequency doubling deep-UV crystals. Nature Communications, 2018, 9, 2972.	5.8	137
104	Nonlinear phononic control and emergent magnetism in Mott insulating titanates. Physical Review B, 2018, 98, .	1.1	31
105	Electronic structure of negative charge transfer CaFeO_3 across the metal-insulator transition. Physical Review Materials, 2018, 2, .	1.8	18
106	Tunable inversion symmetry to control indirect-to-direct band gaps transitions. Physical Review Materials, 2018, 2, .	0.9	4
107	Inducing spontaneous electric polarizations in double perovskite iodide superlattices for ferroelectric photovoltaic materials. Physical Review Materials, 2018, 2, .	0.9	7
108	Effect of fluoropolymer composition on topochemical synthesis of SrMnO_3 F_x oxyfluoride films. Physical Review Materials, 2018, 2, .	0.9	18

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109	Design of a polar half-metallic ferromagnet with accessible and enhanced electric polarization. <i>Physical Review Materials</i> , 2018, 2, .	0.9	6
110	Beryllium-Free $\text{Rb}_2\text{Al}_2\text{B}_2\text{O}_7$ as a Possible Deep-Ultraviolet Nonlinear Optical Material Replacement for $\text{KBe}_2\text{BO}_3\text{F}_2$. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 2969-2973.	7.2	150
111	Beryllium-Free $\text{Rb}_2\text{Al}_2\text{B}_2\text{O}_7$ as a Possible Deep-Ultraviolet Nonlinear Optical Material Replacement for $\text{KBe}_2\text{BO}_3\text{F}_2$. <i>Angewandte Chemie</i> , 2017, 129, 3015-3019.	1.6	72
112	$\text{M}_4\text{Mg}_4(\text{PO}_7)_3$ (M = K, Rb): Structural Engineering of Pyrophosphates for Nonlinear Optical Applications. <i>Chemistry of Materials</i> , 2017, 29, 1845-1855.	3.2	187
113	Learning from data to design functional materials without inversion symmetry. <i>Nature Communications</i> , 2017, 8, 14282.	5.8	76
114	Role of orbital filling on nonlinear ionic Raman scattering in perovskite titanates. <i>Physical Review B</i> , 2017, 95, .	1.1	15
115	Polar Oxides without Inversion Symmetry through Vacancy and Chemical Order. <i>Journal of the American Chemical Society</i> , 2017, 139, 2833-2841.	6.6	34
116	Improved Electrochemical Phase Diagrams from Theory and Experiment: The Ni-Water System and Its Complex Compounds. <i>Journal of Physical Chemistry C</i> , 2017, 121, 9782-9789.	1.5	163
117	Mixed-Metal Carbonate Fluorides as Deep-Ultraviolet Nonlinear Optical Materials. <i>Journal of the American Chemical Society</i> , 2017, 139, 1285-1295.	6.6	195
118	Room Temperature Electric-Field Control of Magnetism in Layered Oxides with Cation Order. <i>Advanced Functional Materials</i> , 2017, 27, 1604312.	7.8	22
119	The Next-Generation of Nonlinear Optical Materials: $\text{Rb}_3\text{Ba}_3\text{Li}_2\text{Al}_4\text{B}_6\text{O}_{20}\text{F}$ Synthesis, Characterization, and Crystal Growth. <i>Advanced Optical Materials</i> , 2017, 5, 1700840.	3.6	68
120	Electrochemical phase diagrams of Ni from <i>ab initio</i> simulations: role of exchange interactions on accuracy. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 475501.	0.7	16
121	Role of 2D and 3D defects on the reduction of LaNiO_3 nanoparticles for catalysis. <i>Scientific Reports</i> , 2017, 7, 10080.	1.6	27
122	<i>A</i> -Site Ordered Double Perovskite $\text{CaMnTi}_2\text{O}_6$ as a Multifunctional Piezoelectric and Ferroelectric Photovoltaic Material. <i>Inorganic Chemistry</i> , 2017, 56, 11854-11861.	1.9	54
123	Rondinelli named 2017 MRS Outstanding Young Investigator for work with complex inorganic oxides. <i>MRS Bulletin</i> , 2017, 42, 321.	1.7	0
124	Nonlinear Optical Materials: The Next-Generation of Nonlinear Optical Materials: $\text{Rb}_3\text{Ba}_3\text{Li}_2\text{Al}_4\text{B}_6\text{O}_{20}\text{F}$ Synthesis, Characterization, and Crystal Growth (<i>Advanced Optical Materials</i> 23/2017). <i>Advanced Optical Materials</i> , 2017, 5, .	3.6	1
125	Tunable band structures in digital oxides with layered crystal habits. <i>Physical Review B</i> , 2017, 96, .	1.1	0
126	Interface-induced phenomena in magnetism. <i>Reviews of Modern Physics</i> , 2017, 89, .	16.4	672

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127	Ferroelectric Oxides with Strong Visible-Light Absorption from Charge Ordering. <i>Chemistry of Materials</i> , 2017, 29, 2445-2451.	3.2	32
128	Interplay of Cation Ordering and Ferroelectricity in Perovskite Tin Iodides: Designing a Polar Halide Perovskite for Photovoltaic Applications. <i>Inorganic Chemistry</i> , 2017, 56, 26-32.	1.9	37
129	Stable MoSi ₂ nanofilms with controllable and high metallicity. <i>Physical Review Materials</i> , 2017, 1, .	0.9	6
130	Informatics-Based Approaches for Accelerated Discovery of Functional Materials. , 2017, , 153-184.		0
131	Comment on "High-pressure synthesis of orthorhombic SrIrO ₃ perovskite and its positive magnetoresistance" [J. Appl. Phys. 103, 103706 (2008)]. <i>Journal of Applied Physics</i> , 2016, 119, 086102.	1.1	6
132	Theory-Guided Machine Learning in Materials Science. <i>Frontiers in Materials</i> , 2016, 3, .	1.2	112
133	Electronic Structure and Band Gap of Fullerenes on Tungsten Surfaces: Transition from a Semiconductor to a Metal Triggered by Annealing. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 34854-34862.	4.0	5
134	Electronic doping of transition metal oxide perovskites. <i>Applied Physics Letters</i> , 2016, 108, .	1.5	5
135	Ultrafast Band Engineering and Transient Spin Currents in Antiferromagnetic Oxides. <i>Scientific Reports</i> , 2016, 6, 25121.	1.6	8
136	Microscopic interactions governing phase matchability in nonlinear optical materials. <i>Journal of Materials Chemistry C</i> , 2016, 4, 5858-5863.	2.7	6
137	Ruddlesden-Popper Hybrid Lead Iodide Perovskite 2D Homologous Semiconductors. <i>Chemistry of Materials</i> , 2016, 28, 2852-2867.	3.2	1,607
138	Polar metals by geometric design. <i>Nature</i> , 2016, 533, 68-72.	13.7	262
139	An efficient ab-initio quasiharmonic approach for the thermodynamics of solids. <i>Computational Materials Science</i> , 2016, 120, 84-93.	1.4	65
140	Tunable Negative Thermal Expansion in Layered Perovskites from Quasi-Two-Dimensional Vibrations. <i>Physical Review Letters</i> , 2016, 117, 115901.	2.9	32
141	Reconstructive Transitions from Rotations of Rigid Heteroanionic Polyhedra. <i>Journal of the American Chemical Society</i> , 2016, 138, 11882-11889.	6.6	13
142	Domain topology and domain switching kinetics in a hybrid improper ferroelectric. <i>Nature Communications</i> , 2016, 7, 11602.	5.8	46
143	Strain-induced nonsymmorphic symmetry breaking and removal of Dirac semimetallic nodal line in an orthoperovskite iridate. <i>Physical Review B</i> , 2016, 93, .	1.1	67
144	Interplay between electron correlations and polar displacements in metallic SrEuMo ₂ O ₆ . <i>Physical Review B</i> , 2016, 93, .	1.1	5

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145	Deep Ultraviolet Nonlinear Optical Materials. Chemistry of Materials, 2016, 28, 5238-5258.	3.2	481
146	Assessing exchange-correlation functional performance for structure and property predictions of oxyfluoride compounds from first principles. Physical Review B, 2016, 94, .	1.1	27
147	Magnetoelectric coupling in the type-I multiferroic ScFeO ₃ . Physical Review B, 2016, 94, .	1.1	13
148	Epitaxial-strain-induced polar-to-nonpolar transitions in layered oxides. Nature Materials, 2016, 15, 951-955.	13.3	94
149	Symmetry-Adapted Distortion Modes as Descriptors for Materials Informatics. Springer Series in Materials Science, 2016, , 213-222.	0.4	3
150	Metals amassing transparency. Nature Materials, 2016, 15, 132-134.	13.3	13
151	Lithium Niobate-Type Oxides as Visible Light Photovoltaic Materials. Chemistry of Materials, 2016, 28, 25-29.	3.2	26
152	Electronic, Crystal Chemistry, and Nonlinear Optical Property Relationships in the Dugganite A ₃ B ₃ CD ₂ O ₁₄ Family. Journal of the American Chemical Society, 2016, 138, 4984-4989.	6.6	118
153	Mismatched lattices patched up. Nature Chemistry, 2016, 8, 292-294.	6.6	14
154	Design of noncentrosymmetric perovskites from centric and acentric basic building units. Journal of Materials Chemistry C, 2016, 4, 4016-4027.	2.7	27
155	Octahedral Rotation Preferences in Perovskite Iodides and Bromides. Journal of Physical Chemistry Letters, 2016, 7, 918-922.	2.1	115
156	Bidenticity-Enhanced Second Harmonic Generation from Pb Chelation in Pb ₃ Mg ₃ TeP ₂ O ₁₄ . Journal of the American Chemical Society, 2016, 138, 88-91.	6.6	143
157	Informatics-Based Approaches for Accelerated Discovery of Functional Materials. Advances in Chemical and Materials Engineering Book Series, 2016, , 192-223.	0.2	2
158	Optical Materials: Design and Synthesis of the Beryllium-Free Deep-Ultraviolet Nonlinear Optical Material Ba ₃ (ZnB ₅ O ₁₀)PO ₄ (Adv. Mater. 45/2015). Advanced Materials, 2015, 27, 7379-7379.	11.1	3
159	Noncentrosymmetric structural transitions in ultrashort ferroelectric A ₂ GaO ₃ /A ₂ GaO ₃ superlattices. Physical Review B, 2015, 91, .	1.1	6
160	Ferroelectricity from coupled cooperative Jahn-Teller distortions and octahedral rotations in ordered Ruddlesden-Popper manganates. Physical Review B, 2015, 92, .	1.1	23
161	Ferroelectricity in double perovskite fluoroscandates. Physical Review B, 2015, 92, .	1.1	1
162	Electrochemical phase diagrams for Ti oxides from density functional calculations. Physical Review B, 2015, 92, .	1.1	35

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163	Design of a Mott Multiferroic from a Nonmagnetic Polar Metal. <i>Physical Review Letters</i> , 2015, 115, 087202.	2.9	64
164	Crystal structure and electronic properties of bulk and thin film brownmillerite oxides. <i>Physical Review B</i> , 2015, 92, .	1.1	67
165	Materials Prediction via Classification Learning. <i>Scientific Reports</i> , 2015, 5, 13285.	1.6	68
166	Design and Synthesis of the Beryllium-Free Deep-Ultraviolet Nonlinear Optical Material $\text{Ba}_3(\text{Zn}_5\text{O}_{10})\text{PO}_4$. <i>Advanced Materials</i> , 2015, 27, 7380-7385.	11.1	262
167	Understanding ferroelectricity in layered perovskites: new ideas and insights from theory and experiments. <i>Dalton Transactions</i> , 2015, 44, 10543-10558.	1.6	218
168	Massive band gap variation in layered oxides through cation ordering. <i>Nature Communications</i> , 2015, 6, 6191.	5.8	36
169	Predicting and Designing Optical Properties of Inorganic Materials. <i>Annual Review of Materials Research</i> , 2015, 45, 491-518.	4.3	56
170	$\text{Pb}_2\text{Ba}_3(\text{BO}_3)_3\text{Cl}$: A Material with Large SHG Enhancement Activated by Pb-Chelated BO_3 Groups. <i>Journal of the American Chemical Society</i> , 2015, 137, 9417-9422.	6.6	255
171	Anharmonic lattice interactions in improper ferroelectrics for multiferroic design. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 283202.	0.7	57
172	Polarization screening-induced magnetic phase gradients at complex oxide interfaces. <i>Nature Communications</i> , 2015, 6, 6735.	5.8	71
173	Tuning the ferroelectric polarization in AA^2MnWO_6 double perovskites through A cation substitution. <i>Dalton Transactions</i> , 2015, 44, 10644-10653.	1.6	29
174	Research Update: Towards designed functionalities in oxide-based electronic materials. <i>APL Materials</i> , 2015, 3, .	2.2	26
175	RbMgCO_3F : A New Beryllium-Free Deep-Ultraviolet Nonlinear Optical Material. <i>Journal of the American Chemical Society</i> , 2015, 137, 10504-10507.	6.6	283
176	Microscopic origin of pressure-induced isosymmetric transitions in fluoromanganate cryolites. <i>Physical Review B</i> , 2014, 90, . Improper ferroelectricity and piezoelectric responses in rhombohedral ($\sqrt{3}\times\sqrt{3}\times 1$) $\text{R}_2\text{Fe}_2\text{O}_7$ perovskite oxides. <i>Physical Review B</i> , 2014, 89, .	1.1	4
177	$\text{Ba}_3(\text{Zn}_5\text{O}_{10})\text{PO}_4$ perovskite oxides. <i>Physical Review B</i> , 2014, 89, .	1.1	20
178	Inductive crystal field control in layered metal oxides with correlated electrons. <i>APL Materials</i> , 2014, 2, .	2.2	12
179	Ferroelectrics: Piezoelectricity Across a Strain-Induced Isosymmetric Ferri-to-Ferroelectric Transition (<i>Adv. Mater. Interfaces</i> 5/2014). <i>Advanced Materials Interfaces</i> , 2014, 1, n/a-n/a.	1.9	1
180	Band structure and optical transitions in LaFeO_3 : theory and experiment. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 505502.	0.7	100

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181	Piezoelectricity Across a Strain-Induced Isosymmetric Ferroelectric Transition. <i>Advanced Materials Interfaces</i> , 2014, 1, 1400042.	1.9	15
182	Designing a robustly metallic noncentrosymmetric ruthenate oxide with large thermopower anisotropy. <i>Nature Communications</i> , 2014, 5, 3432.	5.8	134
183	Inversion Symmetry Breaking by Oxygen Octahedral Rotations in the Ruddlesden-Popper $\text{Na}_x\text{R}_{1-x}\text{TiO}_{3-2x}$. <i>Physical Review Letters</i> , 2014, 112, 187602.	3.9	60
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