

# James M Rondinelli

## List of Publications by Year in Descending Order

**Source:** <https://exaly.com/author-pdf/7424045/james-m-rondinelli-publications-by-year.pdf>

**Version:** 2024-04-17

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

209  
papers

12,476  
citations

55  
h-index

109  
g-index

247  
ext. papers

14,624  
ext. citations

9.1  
avg, IF

6.95  
L-index

#	Paper	IF	Citations
209	Interlayer magnetophononic coupling in MnBiTe. <i>Nature Communications</i> , <b>2022</b> , 13, 1929	17.4	4
208	Perovskite-like KTiOF Exhibits (3 + 1)-Dimensional Commensurate Structure Induced by Octahedrally Coordinated Potassium Ions. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 18907-18916	16.4	0
207	Controlled n-Doping of Naphthalene Diimide-Based Two-Dimensional Polymers. <i>Advanced Materials</i> , <b>2021</b> , e2101932	24	5
206	CuMnGeS and CuMnGeS: two polar thiogermanates exhibiting second harmonic generation in the infrared and structures derived from hexagonal diamond. <i>Dalton Transactions</i> , <b>2021</b> , 50, 17524-17537	4.3	2
205	Structure Tuning, Strong Second Harmonic Generation Response, and High Optical Stability of the Polar Semiconductors NaKAs. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 18204-18215	16.4	3
204	Durable Multimetal Oxochloride Intergrowths for Visible Light-Driven Water Splitting. <i>Chemistry of Materials</i> , <b>2021</b> , 33, 347-358	9.6	6
203	Computationally Directed Discovery of MoBi. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 214-222	17.4	9
202	First-Principles Hydrothermal Synthesis Design to Optimize Conditions and Increase the Yield of Quaternary Heteroanionic Oxochalcogenides. <i>Chemistry of Materials</i> , <b>2021</b> , 33, 2726-2741	9.6	1
201	Local Distortions and Metal-Semiconductor-Metal Transition in Quasi-One-Dimensional Nanowire Compounds AV <sub>3</sub> Q <sub>3</sub> O <sub>4</sub> (A = K, Rb, Cs and Q = Se, Te). <i>Chemistry of Materials</i> , <b>2021</b> , 33, 2611-2623	9.6	1
200	Spectral Addressability in a Modular Two Qubit System. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 8069-8077	16.4	6
199	Negative thermal expansion in the Ruddlesden-Popper calcium titanates. <i>Physical Review Materials</i> , <b>2021</b> , 5,	3.2	1
198	First-Principles-Based Prediction of Electrochemical Oxidation and Corrosion of Copper under Multiple Environmental Factors. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 14027-14038	3.8	2
197	ABX Compounds and the Stabilization of Trirutile Oxides. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 9224-9232	5.1	0
196	Polar Ferromagnetic Metal by Intercalation of Metal-Amine Complexes. <i>Chemistry of Materials</i> , <b>2021</b> , 33, 4936-4947	9.6	1
195	Database, Features, and Machine Learning Model to Identify Thermally Driven Metal-Insulator Transition Compounds. <i>Chemistry of Materials</i> , <b>2021</b> , 33, 5591-5605	9.6	5
194	Physical insights on the low lattice thermal conductivity of AgInSe <sub>2</sub> . <i>Materials Today Physics</i> , <b>2021</b> , 19, 100428	8	9
193	Strain-Induced Anion-Site Occupancy in Perovskite Oxyfluoride Films. <i>Chemistry of Materials</i> , <b>2021</b> , 33, 1811-1820	9.6	6

192	Strain-Induced Magnetic Transitions in SrMO (M = Mn, Fe) Thin Films with Ordered Oxygen Vacancies. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 13161-13167	5.1	
191	Featureless adaptive optimization accelerates functional electronic materials design. <i>Applied Physics Reviews</i> , <b>2020</b> , 7, 041403	17.3	10
190	Synthetic investigation of competing magnetic interactions in 2D metal-chloranilate radical frameworks. <i>Chemical Science</i> , <b>2020</b> , 11, 5922-5928	9.4	6
189	Multimodal Structure Solution with F NMR Crystallography of Spin Singlet Molybdenum Oxyfluorides. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 12288-12298	16.4	6
188	Exploiting Colorimetry for Fidelity in Data Visualization. <i>Chemistry of Materials</i> , <b>2020</b> , 32, 5455-5460	9.6	2
187	Extreme tensile strain states in LaCaMnO membranes. <i>Science</i> , <b>2020</b> , 368, 71-76	33.3	77
186	Anion Ordered and Ferroelectric Ruddlesden-Popper Oxynitride Ca <sub>3</sub> Nb <sub>2</sub> N <sub>2</sub> O <sub>5</sub> for Visible-Light-Active Photocatalysis. <i>Chemistry of Materials</i> , <b>2020</b> , 32, 2815-2823	9.6	12
185	Chemical gradients in human enamel crystallites. <i>Nature</i> , <b>2020</b> , 583, 66-71	50.4	50
184	Uniaxial Strain-Controlled Ground States in Manganite Films. <i>Nano Letters</i> , <b>2020</b> , 20, 1131-1140	11.5	10
183	Ferri-chiral compounds with potentially switchable Dresselhaus spin splitting. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	2
182	Discovery of highly polarizable semiconductors BaZrS <sub>3</sub> and Ba <sub>3</sub> Zr <sub>2</sub> S <sub>7</sub> . <i>Physical Review Materials</i> , <b>2020</b> , 4,	3.2	9
181	Structural signatures of the insulator-to-metal transition in BaCo <sub>1-x</sub> Ni <sub>x</sub> S <sub>2</sub> . <i>Physical Review Materials</i> , <b>2020</b> , 4,	3.2	2
180	Cooperative interactions govern the fermiology of the polar metal Ca <sub>3</sub> Ru <sub>2</sub> O <sub>7</sub> . <i>Physical Review Research</i> , <b>2020</b> , 2,	3.9	7
179	Evidence for an extended critical fluctuation region above the polar ordering transition in LiOsO <sub>3</sub> . <i>Physical Review Research</i> , <b>2020</b> , 2,	3.9	5
178	Design of New Multiferroic Oxides <b>2020</b> , 1151-1212		1
177	Hybrid improper antiferroelectricity—New insights for novel device concepts. <i>MRS Advances</i> , <b>2020</b> , 5, 3521-3545	0.7	1
176	Microscopic Insights into the Reconstructive Phase Transition of KNbO <sub>5</sub> with <sup>19</sup> F NMR Spectroscopy. <i>Chemistry of Materials</i> , <b>2020</b> , 32, 5715-5722	9.6	3
175	Multi-messenger nanoprobe of hidden magnetism in a strained manganite. <i>Nature Materials</i> , <b>2020</b> , 19, 397-404	27	33

174	Discovery Principles and Materials for Symmetry-Protected Persistent Spin Textures with Long Spin Lifetimes. <i>Matter</i> , <b>2020</b> , 3, 1211-1225	12.7	5
173	Persistent polar distortions from covalent interactions in doped BaTiO <sub>3</sub> . <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	8
172	Pressure-Induced Collapse of Magnetic Order in Jarosite. <i>Physical Review Letters</i> , <b>2020</b> , 125, 077202	7.4	0
171	Pressure effects on magnetism in Ca <sub>2</sub> Mn <sub>2</sub> O <sub>5</sub> -type ferrites and manganites. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	1
170	Atomic and electronic structure of domains walls in a polar metal. <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	15
169	Covalency-driven Structural Evolution in the Polar Pyrochlore Series Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> ·xSx. <i>Chemistry of Materials</i> , <b>2019</b> , 31, 7626-7637	9.6	7
168	Catalytic Enhancement of CO Oxidation on LaFeO <sub>3</sub> Regulated by Ruddlesden-Popper Stacking Faults. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 33850-33858	9.5	7
167	Synergistically Optimizing Carrier Concentration and Decreasing Sound Velocity in n-type AgInSe <sub>2</sub> Thermoelectrics. <i>Chemistry of Materials</i> , <b>2019</b> , 31, 8182-8190	9.6	13
166	Predicting the Structure Stability of Layered Heteroanionic Materials Exhibiting Anion Order. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 13229-13240	5.1	5
165	Assessing exchange-correlation functional performance in the chalcogenide lacunar spinels GaM <sub>4</sub> Q <sub>8</sub> (M=Mo, V, Nb, Ta; Q=S,Se). <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	15
164	Physical properties of epitaxial SrMnO <sub>3</sub> F oxyfluoride films. <i>Journal of Physics Condensed Matter</i> , <b>2019</b> , 31, 365602	1.8	3
163	Reliable electrochemical phase diagrams of magnetic transition metals and related compounds from high-throughput ab initio calculations. <i>Npj Materials Degradation</i> , <b>2019</b> , 3,	5.7	18
162	Comprehensive magnetic phase diagrams of the polar metal Ca <sub>3</sub> (Ru <sub>0.95</sub> Fe <sub>0.05</sub> ) <sub>2</sub> O <sub>7</sub> . <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	3
161	Two closely related polymorphs of ammonium trifluorooxovanadate. <i>Journal of Solid State Chemistry</i> , <b>2019</b> , 276, 261-265	3.3	1
160	MnBi <sub>2</sub> : A Metastable High-Pressure Phase in the MnBi System. <i>Chemistry of Materials</i> , <b>2019</b> , 31, 3083-3088	9.6	5
159	Modeling Corrosion with First-Principles Electrochemical Phase Diagrams. <i>Annual Review of Materials Research</i> , <b>2019</b> , 49, 53-77	12.8	30
158	Heteroanionic Materials by Design: Progress Toward Targeted Properties. <i>Advanced Materials</i> , <b>2019</b> , 31, e1805295	24	84
157	Ultrafast quasiparticle dynamics in the correlated semimetal Ca <sub>3</sub> Ru <sub>2</sub> O <sub>7</sub> . <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	2

156	Deliberate Deficiencies: Expanding Electronic Function through Non-stoichiometry. <i>Matter</i> , <b>2019</b> , 1, 33-35.7	5.7	5
155	Property control from polyhedral connectivity in ABO <sub>3</sub> oxides. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	3
154	Symbolic regression in materials science. <i>MRS Communications</i> , <b>2019</b> , 9, 793-805	2.7	40
153	Evidence for the weakly coupled electron mechanism in an Anderson-Blount polar metal. <i>Nature Communications</i> , <b>2019</b> , 10, 3217	17.4	22
152	High-pressure synthesis of the BiVO <sub>3</sub> perovskite. <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	6
151	A-site cation size effect on oxygen octahedral rotations in acentric Ruddlesden-Popper alkali rare-earth titanates. <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	6
150	Uncorrelated Bi off-centering and the insulator-to-metal transition in ruthenium A <sub>2</sub> Ru <sub>2</sub> O <sub>7</sub> pyrochlores. <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	8
149	Understanding Electrochemical Stabilities of Ni-Based Nanofilms from a Comparative TheoryExperiment Approach. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 28925-28940	3.8	4
148	Design of Heteroanionic MoON Exhibiting a Peierls Metal-Insulator Transition. <i>Physical Review Letters</i> , <b>2019</b> , 123, 236402	7.4	7
147	Design of New Multiferroic Oxides <b>2019</b> , 1-62		
146	Anisotropic magnetoresistance in the itinerant antiferromagnetic EuTiO <sub>3</sub> . <i>Physical Review B</i> , <b>2019</b> , 99,	3.3	21
145	Pb BO I: A Borate Iodide with the Largest Second-Harmonic Generation (SHG) Response in the KBe BO F (KBBF) Family of Nonlinear Optical (NLO) Materials. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 6100-6103	16.4	125
144	Pb <sub>2</sub> BO <sub>3</sub> I: A Borate Iodide with the Largest Second-Harmonic Generation (SHG) Response in the KBe <sub>2</sub> BO <sub>3</sub> F <sub>2</sub> (KBBF) Family of Nonlinear Optical (NLO) Materials. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 6208-6211	3.6	22
143	Crystal structure stability and electronic properties of the layered nickelate La <sub>4</sub> Ni <sub>3</sub> O <sub>10</sub> . <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	6
142	Expanding frontiers in materials chemistry and physics with multiple anions. <i>Nature Communications</i> , <b>2018</b> , 9, 772	17.4	379
141	Observation of Quasi-Two-Dimensional Polar Domains and Ferroelastic Switching in a Metal, CaRuO. <i>Nano Letters</i> , <b>2018</b> , 18, 3088-3095	11.5	39
140	Tunable metal-insulator transition, Rashba effect and Weyl Fermions in a relativistic charge-ordered ferroelectric oxide. <i>Nature Communications</i> , <b>2018</b> , 9, 492	17.4	24
139	Structural Diversity from Anion Order in Heteroanionic Materials. <i>Chemistry of Materials</i> , <b>2018</b> , 30, 3528-3537	3.5	24

138	Localized Symmetry Breaking for Tuning Thermal Expansion in ScF Nanoscale Frameworks. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 4477-4480	16.4	26
137	The must-have and nice-to-have experimental and computational requirements for functional frequency doubling deep-UV crystals. <i>Nature Communications</i> , <b>2018</b> , 9, 2972	17.4	70
136	Nonlinear phononic control and emergent magnetism in Mott insulating titanates. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	17
135	Electronic structure of negative charge transfer CaFeO <sub>3</sub> across the metal-insulator transition. <i>Physical Review Materials</i> , <b>2018</b> , 2,	3.2	18
134	Tunable inversion symmetry to control indirect-to-direct band gaps transitions. <i>Physical Review Materials</i> , <b>2018</b> , 2,	3.2	3
133	Inducing spontaneous electric polarizations in double perovskite iodide superlattices for ferroelectric photovoltaic materials. <i>Physical Review Materials</i> , <b>2018</b> , 2,	3.2	5
132	Effect of fluoropolymer composition on topochemical synthesis of SrMnO <sub>3</sub> Fluoride films. <i>Physical Review Materials</i> , <b>2018</b> , 2,	3.2	15
131	Design of a polar half-metallic ferromagnet with accessible and enhanced electric polarization. <i>Physical Review Materials</i> , <b>2018</b> , 2,	3.2	4
130	Polar metals as electrodes to suppress the critical-thickness limit in ferroelectric nanocapacitors. <i>Journal of Applied Physics</i> , <b>2018</b> , 124, 174102	2.5	16
129	Structure Dependent Phase Stability and Thermal Expansion of Ruddlesden-Popper Strontium Titanates. <i>Chemistry of Materials</i> , <b>2018</b> , 30, 7100-7110	9.6	10
128	Linear and nonlinear optical probe of the ferroelectric-like phase transition in a polar metal, LiOsO <sub>3</sub> . <i>Applied Physics Letters</i> , <b>2018</b> , 113, 122906	3.4	18
127	Hybrid Improper Ferroelectricity in (Sr,Ca)SnO and Beyond: Universal Relationship between Ferroelectric Transition Temperature and Tolerance Factor in n = 2 Ruddlesden-Popper Phases. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 15690-15700	16.4	45
126	Coupled Raman-Raman modes in the ionic Raman scattering process. <i>Applied Physics Letters</i> , <b>2018</b> , 113, 112903	3.4	1
125	Discovery of Cu <sub>3</sub> Pb. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 12991-12995	3.6	2
124	Discovery of CuPb. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 12809-12813	16.4	3
123	Learning from Correlations Based on Local Structure: Rare-Earth Nickelates Revisited. <i>Journal of Chemical Information and Modeling</i> , <b>2018</b> , 58, 2491-2501	6.1	6
122	Ferroelectric Sr <sub>3</sub> Zr <sub>2</sub> O <sub>7</sub> : Competition between Hybrid Improper Ferroelectric and Antiferroelectric Mechanisms. <i>Advanced Functional Materials</i> , <b>2018</b> , 28, 1801856	15.6	57
121	Understanding Chemical Bonding in Alloys and the Representation in Atomistic Simulations. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 14996-15009	3.8	19

120	Beryllium-Free $\text{RbAlBO}_3$ 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> , <b>2017</b> , 56, 2969-2973	16.4	110
119	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> , <b>2017</b> , 129, 3015-3019	3.6	64
118	$\text{M}_4\text{Mg}_4(\text{P}_2\text{O}_7)_3$ (M = K, Rb): Structural Engineering of Pyrophosphates for Nonlinear Optical Applications. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 1845-1855	9.6	121
117	Learning from data to design functional materials without inversion symmetry. <i>Nature Communications</i> , <b>2017</b> , 8, 14282	17.4	55
116	Role of orbital filling on nonlinear ionic Raman scattering in perovskite titanates. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	10
115	Polar Oxides without Inversion Symmetry through Vacancy and Chemical Order. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 2833-2841	16.4	27
114	Improved Electrochemical Phase Diagrams from Theory and Experiment: The $\text{Ni}/\text{Water}$ System and Its Complex Compounds. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 9782-9789	3.8	92
113	Mixed-Metal Carbonate Fluorides as Deep-Ultraviolet Nonlinear Optical Materials. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 1285-1295	16.4	130
112	Room Temperature Electric-Field Control of Magnetism in Layered Oxides with Cation Order. <i>Advanced Functional Materials</i> , <b>2017</b> , 27, 1604312	15.6	17
111	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> , <b>2017</b> , 5, 1700840	8.1	52
110	Electrochemical phase diagrams of Ni from ab initio simulations: role of exchange interactions on accuracy. <i>Journal of Physics Condensed Matter</i> , <b>2017</b> , 29, 475501	1.8	10
109	Role of 2D and 3D defects on the reduction of $\text{LaNiO}$ nanoparticles for catalysis. <i>Scientific Reports</i> , <b>2017</b> , 7, 10080	4.9	21
108	A-Site Ordered Double Perovskite $\text{CaMnTiO}$ as a Multifunctional Piezoelectric and Ferroelectric-Photovoltaic Material. <i>Inorganic Chemistry</i> , <b>2017</b> , 56, 11854-11861	5.1	33
107	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 (Advanced Optical Materials 23/2017). <i>Advanced Optical Materials</i> , <b>2017</b> , 5,	8.1	1
106	Interface-Induced Phenomena in Magnetism. <i>Reviews of Modern Physics</i> , <b>2017</b> , 89,	40.5	475
105	Ferroelectric Oxides with Strong Visible-Light Absorption from Charge Ordering. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 2445-2451	9.6	24
104	Interplay of Cation Ordering and Ferroelectricity in Perovskite Tin Iodides: Designing a Polar Halide Perovskite for Photovoltaic Applications. <i>Inorganic Chemistry</i> , <b>2017</b> , 56, 26-32	5.1	27
103	Stable $\text{MoSi}_2$ nanofilms with controllable and high metallicity. <i>Physical Review Materials</i> , <b>2017</b> , 1,	3.2	3



102 Informatics-Based Approaches for Accelerated Discovery of Functional Materials **2017**, 153-184

101	Reconstructive Transitions from Rotations of Rigid Heteroanionic Polyhedra. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 11882-9	16.4	7
100	Domain topology and domain switching kinetics in a hybrid improper ferroelectric. <i>Nature Communications</i> , <b>2016</b> , 7, 11602	17.4	35
99	Strain-induced nonsymmorphic symmetry breaking and removal of Dirac semimetallic nodal line in an orthoperovskite iridate. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	60
98	Interplay between electron correlations and polar displacements in metallic SrEuMo <sub>2</sub> O <sub>6</sub> . <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	4
97	Deep Ultraviolet Nonlinear Optical Materials. <i>Chemistry of Materials</i> , <b>2016</b> , 28, 5238-5258	9.6	353
96	Assessing exchange-correlation functional performance for structure and property predictions of oxyfluoride compounds from first principles. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	22
95	Magnetoelectric coupling in the type-I multiferroic ScFeO <sub>3</sub> . <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	6
94	Epitaxial-strain-induced polar-to-nonpolar transitions in layered oxides. <i>Nature Materials</i> , <b>2016</b> , 15, 951-57	65	
93	Symmetry-Adapted Distortion Modes as Descriptors for Materials Informatics. <i>Springer Series in Materials Science</i> , <b>2016</b> , 213-222	0.9	2
92	Correlated oxides: Metals amassing transparency. <i>Nature Materials</i> , <b>2016</b> , 15, 132-4	27	10
91	Lithium Niobate-Type Oxides as Visible Light Photovoltaic Materials. <i>Chemistry of Materials</i> , <b>2016</b> , 28, 25-29	9.6	24
90	Electronic, Crystal Chemistry, and Nonlinear Optical Property Relationships in the Dugganite A <sub>3</sub> B <sub>3</sub> CD <sub>2</sub> O <sub>14</sub> Family. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 4984-9	16.4	89
89	Oxide interfaces: Mismatched lattices patched up. <i>Nature Chemistry</i> , <b>2016</b> , 8, 292-4	17.6	10
88	Design of noncentrosymmetric perovskites from centric and acentric basic building units. <i>Journal of Materials Chemistry C</i> , <b>2016</b> , 4, 4016-4027	7.1	25
87	Octahedral Rotation Preferences in Perovskite Iodides and Bromides. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 918-22	6.4	84
86	Bidenticity-Enhanced Second Harmonic Generation from Pb Chelation in Pb <sub>3</sub> Mg <sub>3</sub> TeP <sub>2</sub> O <sub>14</sub> . <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 88-91	16.4	112
85	Informatics-Based Approaches for Accelerated Discovery of Functional Materials. <i>Advances in Chemical and Materials Engineering Book Series</i> , <b>2016</b> , 192-223	0.2	2



84	Comment on High-pressure synthesis of orthorhombic SrIrO <sub>3</sub> perovskite and its positive magnetoresistance [J. Appl. Phys. 103, 103706 (2008)]. <i>Journal of Applied Physics</i> , <b>2016</b> , 119, 086102	2.5	5
83	Theory-Guided Machine Learning in Materials Science. <i>Frontiers in Materials</i> , <b>2016</b> , 3,	4	76
82	Electronic Structure and Band Gap of Fullerenes on Tungsten Surfaces: Transition from a Semiconductor to a Metal Triggered by Annealing. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2016</b> , 8, 34854-34862	2.5	5
81	Electronic doping of transition metal oxide perovskites. <i>Applied Physics Letters</i> , <b>2016</b> , 108, 213109	3.4	3
80	Ultrafast Band Engineering and Transient Spin Currents in Antiferromagnetic Oxides. <i>Scientific Reports</i> , <b>2016</b> , 6, 25121	4.9	5
79	Microscopic interactions governing phase matchability in nonlinear optical materials. <i>Journal of Materials Chemistry C</i> , <b>2016</b> , 4, 5858-5863	7.1	5
78	Ruddlesden-Popper Hybrid Lead Iodide Perovskite 2D Homologous Semiconductors. <i>Chemistry of Materials</i> , <b>2016</b> , 28, 2852-2867	9.6	1166
77	Polar metals by geometric design. <i>Nature</i> , <b>2016</b> , 533, 68-72	50.4	203
76	An efficient ab-initio quasiharmonic approach for the thermodynamics of solids. <i>Computational Materials Science</i> , <b>2016</b> , 120, 84-93	3.2	43
75	Tunable Negative Thermal Expansion in Layered Perovskites from Quasi-Two-Dimensional Vibrations. <i>Physical Review Letters</i> , <b>2016</b> , 117, 115901	7.4	20
74	Predicting and Designing Optical Properties of Inorganic Materials. <i>Annual Review of Materials Research</i> , <b>2015</b> , 45, 491-518	12.8	45
73	Pb <sub>2</sub> Ba <sub>3</sub> (BO <sub>3</sub> ) <sub>3</sub> Cl: A Material with Large SHG Enhancement Activated by Pb-Chelated BO <sub>3</sub> Groups. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 9417-22	16.4	220
72	Anharmonic lattice interactions in improper ferroelectrics for multiferroic design. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 283202	1.8	44
71	Polarization screening-induced magnetic phase gradients at complex oxide interfaces. <i>Nature Communications</i> , <b>2015</b> , 6, 6735	17.4	64
70	Tuning the ferroelectric polarization in AA'MnWO <sub>6</sub> double perovskites through A cation substitution. <i>Dalton Transactions</i> , <b>2015</b> , 44, 10644-53	4.3	25
69	Research Update: Towards designed functionalities in oxide-based electronic materials. <i>APL Materials</i> , <b>2015</b> , 3, 080702	5.7	23
68	RbMgCO <sub>3</sub> : A New Beryllium-Free Deep-Ultraviolet Nonlinear Optical Material. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 10504-7	16.4	209
67	Optical Materials: Design and Synthesis of the Beryllium-Free Deep-Ultraviolet Nonlinear Optical Material Ba <sub>3</sub> (ZnB <sub>5</sub> O <sub>10</sub> )PO <sub>4</sub> (Adv. Mater. 45/2015). <i>Advanced Materials</i> , <b>2015</b> , 27, 7379-7379	24	3

66	Noncentrosymmetric structural transitions in ultrashort ferroelectric A <sub>2</sub> GaO <sub>3</sub> /A <sub>2</sub> GaO <sub>3</sub> superlattices. <i>Physical Review B</i> , <b>2015</b> , 91,	3-3	5
65	Ferroelectricity from coupled cooperative Jahn-Teller distortions and octahedral rotations in ordered Ruddlesden-Popper manganates. <i>Physical Review B</i> , <b>2015</b> , 92,	3-3	19
64	Ferroelectricity in d <sup>0</sup> double perovskite fluoroscandates. <i>Physical Review B</i> , <b>2015</b> , 92,	3-3	1
63	Electrochemical phase diagrams for Ti oxides from density functional calculations. <i>Physical Review B</i> , <b>2015</b> , 92,	3-3	31
62	Design of a Mott Multiferroic from a Nonmagnetic Polar Metal. <i>Physical Review Letters</i> , <b>2015</b> , 115, 087202	4	50
61	Crystal structure and electronic properties of bulk and thin film brownmillerite oxides. <i>Physical Review B</i> , <b>2015</b> , 92,	3-3	53
60	Materials Prediction via Classification Learning. <i>Scientific Reports</i> , <b>2015</b> , 5, 13285	4-9	65
59	Design and Synthesis of the Beryllium-Free Deep-Ultraviolet Nonlinear Optical Material Ba <sub>2</sub> (ZnBO <sub>4</sub> ) <sub>2</sub> PO <sub>4</sub> . <i>Advanced Materials</i> , <b>2015</b> , 27, 7380-5	24	208
58	Understanding ferroelectricity in layered perovskites: new ideas and insights from theory and experiments. <i>Dalton Transactions</i> , <b>2015</b> , 44, 10543-58	4-3	159
57	Massive band gap variation in layered oxides through cation ordering. <i>Nature Communications</i> , <b>2015</b> , 6, 6191	17.4	27
56	Designing a robustly metallic noncentrosymmetric ruthenate oxide with large thermopower anisotropy. <i>Nature Communications</i> , <b>2014</b> , 5, 3432	17.4	105
55	Inversion symmetry breaking by oxygen octahedral rotations in the Ruddlesden-Popper NaRTiO <sub>4</sub> family. <i>Physical Review Letters</i> , <b>2014</b> , 112, 187602	7-4	45
54	Estimating Hybridization of Transition Metal and Oxygen States in Perovskites from O K-edge X-ray Absorption Spectroscopy. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 1856-1863	3.8	244
53	Crystal-chemistry guidelines for noncentrosymmetric A <sub>2</sub> BO <sub>4</sub> Ruddlesden-Popper oxides. <i>Inorganic Chemistry</i> , <b>2014</b> , 53, 336-48	5-1	64
52	Covalent dependence of octahedral rotations in orthorhombic perovskite oxides. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 114704	3-9	52
51	Role of acentric displacements on the crystal structure and second-harmonic generating properties of RbPbCO <sub>3</sub> F and CsPbCO <sub>3</sub> F. <i>Inorganic Chemistry</i> , <b>2014</b> , 53, 6241-51	5-1	75
50	Effect of interfacial octahedral behavior in ultrathin manganite films. <i>Nano Letters</i> , <b>2014</b> , 14, 2509-14	11.5	109
49	Electronically driven structural transitions in A <sub>10</sub> (PO <sub>4</sub> ) <sub>6</sub> F <sub>2</sub> apatites (A = Ca, Sr, Pb, Cd and Hg). <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , <b>2014</b> , 70, 612-5	1.8	11

48	Colloquium: Emergent properties in plane view: Strong correlations at oxide interfaces. <i>Reviews of Modern Physics</i> , <b>2014</b> , 86, 1189-1202	40.5	207
47	Microscopic Origins of Optical Second Harmonic Generation in Noncentrosymmetric Nonpolar Materials. <i>Chemistry of Materials</i> , <b>2014</b> , 26, 5773-5781	9.6	63
46	Contributions of Correlated Acentric Atomic Displacements to the Nonlinear Second Harmonic Generation and Response. <i>ACS Photonics</i> , <b>2014</b> , 1, 96-100	6.3	20
45	Linear optical and electronic properties of the polar metallic ruthenate (Sr,Ca)Ru <sub>2</sub> O <sub>6</sub> . <i>Journal of Physics Condensed Matter</i> , <b>2014</b> , 26, 265501	1.8	2
44	Polar Cation Ordering: A Route to Introducing >10% Bond Strain Into Layered Oxide Films. <i>Advanced Functional Materials</i> , <b>2014</b> , 24, 6884-6891	15.6	19
43	Thickness-dependent crossover from charge- to strain-mediated magnetoelectric coupling in ferromagnetic/piezoelectric oxide heterostructures. <i>ACS Nano</i> , <b>2014</b> , 8, 894-903	16.7	54
42	Cs <sub>3</sub> Zn <sub>6</sub> B <sub>9</sub> O <sub>21</sub> : a chemically benign member of the KBBF family exhibiting the largest second harmonic generation response. <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 1264-7	16.4	273
41	Microscopic origin of pressure-induced isosymmetric transitions in fluoromanganate cryolites. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	4
40	Improper ferroelectricity and piezoelectric responses in rhombohedral (A,A')B <sub>2</sub> O <sub>6</sub> perovskite oxides. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	16
39	Inductive crystal field control in layered metal oxides with correlated electrons. <i>APL Materials</i> , <b>2014</b> , 2, 076110	5.7	11
38	Ferroelectrics: Piezoelectricity Across a Strain-Induced Isosymmetric Ferri-to-Ferroelectric Transition (Adv. Mater. Interfaces 5/2014). <i>Advanced Materials Interfaces</i> , <b>2014</b> , 1, n/a-n/a	4.6	1
37	Band structure and optical transitions in LaFeO <sub>3</sub> : theory and experiment. <i>Journal of Physics Condensed Matter</i> , <b>2014</b> , 26, 505502	1.8	71
36	Piezoelectricity Across a Strain-Induced Isosymmetric Ferri-to-Ferroelectric Transition. <i>Advanced Materials Interfaces</i> , <b>2014</b> , 1, 1400042	4.6	15
35	Interplay of octahedral rotations and breathing distortions in charge-ordering perovskite oxides. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	62
34	Heterointerface engineered electronic and magnetic phases of NdNiO <sub>3</sub> thin films. <i>Nature Communications</i> , <b>2013</b> , 4, 2714	17.4	136
33	Atomic Scale Design of Polar Perovskite Oxides without Second-Order Jahn-Teller Ions. <i>Chemistry of Materials</i> , <b>2013</b> , 25, 4545-4550	9.6	39
32	Octahedral engineering of orbital polarizations in charge transfer oxides. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	23
31	Designing a deep-ultraviolet nonlinear optical material with a large second harmonic generation response. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 4215-8	16.4	466

30	Normal mode determination of perovskite crystal structures with octahedral rotations: theory and applications. <i>Journal of Physics Condensed Matter</i> , <b>2013</b> , 25, 175902	1.8	49
29	Interplay of octahedral tilts and polar order in BiFeO <sub>3</sub> films. <i>Advanced Materials</i> , <b>2013</b> , 25, 2497-504	24	94
28	Turning ABO <sub>3</sub> Antiferroelectrics into Ferroelectrics: Design Rules for Practical Rotation-Driven Ferroelectricity in Double Perovskites and A <sub>3</sub> B <sub>2</sub> O <sub>7</sub> Ruddlesden-Popper Compounds. <i>Advanced Functional Materials</i> , <b>2013</b> , 23, n/a-n/a	15.6	98
27	Connecting bulk symmetry and orbital polarization in strained RNiO <sub>3</sub> ultrathin films. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	33
26	Correlation effects and spin-orbit interactions in two-dimensional hexagonal 5d transition metal carbides, Ta <sub>n+1</sub> C <sub>n</sub> (n = 1,2,3). <i>Europhysics Letters</i> , <b>2013</b> , 101, 57004	1.6	43
25	Control of octahedral connectivity in perovskite oxide heterostructures: An emerging route to multifunctional materials discovery. <i>MRS Bulletin</i> , <b>2012</b> , 37, 261-270	3.2	324
24	Whither the oxide interface. <i>Nature Materials</i> , <b>2012</b> , 11, 92-4	27	247
23	Spin-assisted covalent bond mechanism in charge-ordering perovskite oxides. <i>Physical Review B</i> , <b>2012</b> , 86,	3.3	20
22	Strain-controlled band engineering and self-doping in ultrathin LaNiO <sub>3</sub> films. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	30
21	Octahedral rotation-induced ferroelectricity in cation ordered perovskites. <i>Advanced Materials</i> , <b>2012</b> , 24, 1961-8	24	245
20	Ferroelectricity: Octahedral Rotation-Induced Ferroelectricity in Cation Ordered Perovskites (Adv. Mater. 15/2012). <i>Advanced Materials</i> , <b>2012</b> , 24, 1918-1918	24	11
19	Large isosymmetric reorientation of oxygen octahedra rotation axes in epitaxially strained perovskites. <i>Physical Review Letters</i> , <b>2011</b> , 106, 235502	7.4	42
18	Lattice normal modes and electronic properties of the correlated metal LaNiO <sub>3</sub> . <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	98
17	First-principles study of misfit strain-stabilized ferroelectric SnTiO <sub>3</sub> . <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	42
16	Structure and properties of functional oxide thin films: insights from electronic-structure calculations. <i>Advanced Materials</i> , <b>2011</b> , 23, 3363-81	24	284
15	K <sub>3</sub> B <sub>6</sub> O <sub>10</sub> Cl: a new structure analogous to perovskite with a large second harmonic generation response and deep UV absorption edge. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 7786-90	16.4	540
14	Asymmetric orbital-lattice interactions in ultrathin correlated oxide films. <i>Physical Review Letters</i> , <b>2011</b> , 107, 116805	7.4	142
13	Quantifying octahedral rotations in strained perovskite oxide films. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	264

12	Electron-lattice instabilities suppress cuprate-like electronic structures in SrFeO <sub>3</sub> /SrTiO <sub>3</sub> superlattices. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	20
11	Substrate coherency driven octahedral rotations in perovskite oxide films. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	84
10	Non-d <sup>0</sup> Mn-driven ferroelectricity in antiferromagnetic BaMnO <sub>3</sub> . <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	142
9	Structural effects on the spin-state transition in epitaxially strained LaCoO <sub>3</sub> films. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	81
8	Carrier-mediated magnetoelectricity in complex oxide heterostructures. <i>Nature Nanotechnology</i> , <b>2008</b> , 3, 46-50	28.7	284
7	Electronic properties of bulk and thin film SrRuO <sub>3</sub> : Search for the metal-insulator transition. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	124
6	Charge defects glowing in the dark. <i>Ultramicroscopy</i> , <b>2007</b> , 107, 374-81	3.1	8
5	Surface Reconstruction with a Fractional Hole: (sqrt[5] x sqrt[5])R26.6 degrees LaAlO <sub>3</sub> (001). <i>Physical Review Letters</i> , <b>2007</b> , 98, 086102	7.4	43
4	Enhancing structure relaxations for first-principles codes: An approximate Hessian approach. <i>Computational Materials Science</i> , <b>2007</b> , 40, 345-353	3.2	10
3	Spectral manipulation in Fabry-Perot lasers: perturbative inverse scattering approach. <i>Journal of the Optical Society of America B: Optical Physics</i> , <b>2006</b> , 23, 1046	1.7	23
2	Three-Dimensionally Ordered Macroporous Li <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub> : Effect of Wall Structure on Electrochemical Properties. <i>Chemistry of Materials</i> , <b>2006</b> , 18, 482-489	9.6	271
1	Giant Non-Resonant Infrared Second Order Nonlinearity in $\beta$ -NaAsSe <sub>2</sub> . <i>Advanced Optical Materials</i> , <b>2017</b> , 9, 1700029	2.9	3