

Andrew M Rappe

List of Publications by Year in Descending Order

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

293
papers

21,456
citations

72
h-index

140
g-index

307
ext. papers

24,589
ext. citations

8.6
avg, IF

7.21
L-index

#	Paper	IF	Citations
293	Intrinsic Fermi-surface contribution to the bulk photovoltaic effect. <i>Physical Review Research</i> , 2021 , 3,	3.9	3
292	Mechanistic Study of the Li-Air Battery with a Co ₃ O ₄ Cathode and Dimethyl Sulfoxide Electrolyte. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 21873-21881	3.8	2
291	Hydrogen freedom linked to perovskite efficiency. <i>Nature Materials</i> , 2021 , 20, 914-915	27	
290	Phonon-Assisted Ballistic Current from First-Principles Calculations. <i>Physical Review Letters</i> , 2021 , 126, 177403	7.4	8
289	Widespread Negative Longitudinal Piezoelectric Responses in Ferroelectric Crystals with Layered Structures. <i>Physical Review Letters</i> , 2021 , 126, 217601	7.4	7
288	Strongly Anharmonic Octahedral Tilting in Two-Dimensional Hybrid Halide Perovskites. <i>ACS Nano</i> , 2021 , 15, 10153-10162	16.7	15
287	The Significance of Polarons and Dynamic Disorder in Halide Perovskites. <i>ACS Energy Letters</i> , 2021 , 6, 2162-2173	20.1	17
286	Comprehensive defect suppression in perovskite nanocrystals for high-efficiency light-emitting diodes. <i>Nature Photonics</i> , 2021 , 15, 148-155	33.9	257
285	Metal cation s lone-pairs increase octahedral tilting instabilities in halide perovskites. <i>Materials Advances</i> , 2021 , 2, 4610-4616	3.3	6
284	Large Bulk Piezophotovoltaic Effect of Monolayer 2-MoS. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 1244-1249	6.4	11
283	Oxygen-Initiated Free-Radical Polymerization of Alkyl Acrylates at High Temperatures. <i>Macromolecules</i> , 2021 , 54, 7925-7930	5.5	0
282	Mechanistic Insights into CO ₂ Electroreduction on Ni ₂ P: Understanding Its Selectivity toward Multicarbon Products. <i>ACS Catalysis</i> , 2021 , 11, 11706-11715	13.1	8
281	Stromataxic Stabilization of a Metastable Layered ScFeO ₃ Polymorph. <i>Chemistry of Materials</i> , 2021 , 33, 7423-7431	9.6	1
280	Kinetically Stable Oxide Overlayers on Mo P Nanoparticles Enabling Lithium-Air Batteries with Low Overpotentials and Long Cycle Life. <i>Advanced Materials</i> , 2020 , 32, e2004028	24	14
279	General Approach for Reducing Continuous Translational Symmetry Errors in Finite Difference Real-Space Calculations. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 4327-4336	6.4	
278	Unraveling the Elastic Properties of (Quasi)Two-Dimensional Hybrid Perovskites: A Joint Experimental and Theoretical Study. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 17881-17892	9.5	10
277	Ideal near-Dirac triple-point semimetal in III-V semiconductor alloys. <i>Physical Review B</i> , 2020 , 101,	3.3	3

276	Origin of the anomalous Pb-Br bond dynamics in formamidinium lead bromide perovskites. <i>Physical Review B</i> , 2020 , 101,	3.3	7
275	Shift-current bulk photovoltaic effect influenced by quasiparticle and exciton. <i>Physical Review B</i> , 2020 , 101,	3.3	21
274	Large-area epitaxial growth of curvature-stabilized ABC trilayer graphene. <i>Nature Communications</i> , 2020 , 11, 546	17.4	25
273	Lattice mode symmetry analysis of the orthorhombic phase of methylammonium lead iodide using polarized Raman. <i>Physical Review Materials</i> , 2020 , 4,	3.2	8
272	Elucidating the atomistic origin of anharmonicity in tetragonal CH ₃ NH ₃ PbI ₃ with Raman scattering. <i>Physical Review Materials</i> , 2020 , 4,	3.2	18
271	A Robust and Unified Solution for Choosing the Phases of Adiabatic States as a Function of Geometry: Extending Parallel Transport Concepts to the Cases of Trivial and Near-Trivial Crossings. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 835-846	6.4	2
270	Experimental and Mechanistic Modeling Study of Self-Initiated High-Temperature Polymerization of Ethyl Acrylate. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 2621-2630	3.9	8
269	Optical signatures of multifold fermions in the chiral topological semimetal CoSi. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 27104-27110	11.5	10
268	Impact of Hierarchical Nanoporous Architectures on Sodium Storage in Antimony-Based Sodium-Ion Battery Anodes. <i>ACS Applied Energy Materials</i> , 2020 , 3, 11231-11241	6.1	4
267	Ferroelectric Switching of Pure Spin Polarization in Two-Dimensional Electron Gas. <i>Nano Letters</i> , 2020 , 20, 7230-7236	11.5	1
266	Shift photovoltaic current and magnetically induced bulk photocurrent in piezoelectric sillenite crystals. <i>Physical Review B</i> , 2020 , 102,	3.3	8
265	Epitaxial TiO _x Surface in Ferroelectric BaTiO ₃ : Native Structure and Dynamic Patterning at the Atomic Scale. <i>Advanced Functional Materials</i> , 2020 , 30, 1902549	15.6	10
264	Surface Pyroelectricity in Cubic SrTiO. <i>Advanced Materials</i> , 2019 , 31, e1904733	24	29
263	Mechanochemical Effects of Adsorbates at Nanoelectromechanical Switch Contacts. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 39238-39247	9.5	2
262	Terahertz field-induced ferroelectricity in quantum paraelectric SrTiO. <i>Science</i> , 2019 , 364, 1079-1082	33.3	129
261	Kinetic control of tunable multi-state switching in ferroelectric thin films. <i>Nature Communications</i> , 2019 , 10, 1282	17.4	28
260	Water in hybrid perovskites: Bulk MAPbI ₃ degradation via super-hydrous state. <i>APL Materials</i> , 2019 , 7, 041112	5.7	25
259	Epitaxial Strain Control of Relaxor Ferroelectric Phase Evolution. <i>Advanced Materials</i> , 2019 , 31, e1901060	14	20

258	Bioferroelectric Properties of Glycine Crystals. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 1319-1324	6.4	17
257	Theoretical Insights Into Thermal Self-Initiation Reactions of Acrylates 2019 , 99-134		0
256	Theoretical Insights Into Chain Transfer Reactions of Acrylates 2019 , 135-193		
255	Predicting synthesizability. <i>Journal Physics D: Applied Physics</i> , 2019 , 52,	3	161
254	Upper limit on shift current generation in extended systems. <i>Physical Review B</i> , 2019 , 100,	3-3	11
253	Spatially dispersive circular photogalvanic effect in a Weyl semimetal. <i>Nature Materials</i> , 2019 , 18, 955-962	7	58
252	Breakdown of the Static Picture of Defect Energetics in Halide Perovskites: The Case of the Br Vacancy in CsPbBr ₃ . <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 4490-4498	6.4	25
251	Topological Semimetals from First Principles. <i>Annual Review of Materials Research</i> , 2019 , 49, 153-183	12.8	67
250	Method of Moments Applied to Most-Likely High-Temperature Free-Radical Polymerization Reactions. <i>Processes</i> , 2019 , 7, 656	2.9	7
249	Ferroelectric barium titanate derivatives containing Mo and Mg for transparent photovoltaic applications. <i>Journal of Applied Physics</i> , 2019 , 126, 174101	2.5	4
248	Sr-induced dipole scatter in Ba _x Sr _{1-x} TiO ₃ : Insights from a transferable-bond valence-based interatomic potential. <i>Physical Review B</i> , 2019 , 100,	3-3	7
247	In Situ Bottom-up Synthesis of Porphyrin-Based Covalent Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2019 , 141, 19560-19564	16.4	29
246	Mix and Match: Organic and Inorganic Ions in the Perovskite Lattice. <i>Advanced Materials</i> , 2019 , 31, e1802697	2.9	23
245	Automatic Prediction of Surface Phase Diagrams Using Ab Initio Grand Canonical Monte Carlo. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 2321-2328	3.8	26
244	Effect of wavefunction delocalization on shift current generation. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 084002	1.8	5
243	Big data approach for effective ionic radii. <i>Computer Physics Communications</i> , 2019 , 237, 238-243	4.2	4
242	Spin-orbit enhanced carrier lifetimes in noncentrosymmetric semiconductors. <i>Journal of Physics and Chemistry of Solids</i> , 2019 , 128, 225-230	3.9	1
241	Crystalline Bilayer Graphene with Preferential Stacking from Ni-Cu Gradient Alloy. <i>ACS Nano</i> , 2018 , 12, 2275-2282	16.7	32

240	Molecule-Adsorbed Topological Insulator and Metal Surfaces: A Comparative First-Principles Study. <i>Chemistry of Materials</i> , 2018 , 30, 1849-1855	9.6	6
239	Climbing the Volcano of Electrocatalytic Activity while Avoiding Catalyst Corrosion: Ni ₃ P, a Hydrogen Evolution Electrocatalyst Stable in Both Acid and Alkali. <i>ACS Catalysis</i> , 2018 , 8, 4408-4419	13.1	117
238	Hybrid functional pseudopotentials. <i>Physical Review B</i> , 2018 , 97,	3.3	13
237	Mixed Valence Perovskite Cs Au I : A Potential Material for Thin-Film Pb-Free Photovoltaic Cells with Ultrahigh Efficiency. <i>Advanced Materials</i> , 2018 , 30, e1707001	24	54
236	Anion Exchange in II-VI Semiconducting Nanostructures via Atomic Templating. <i>Nano Letters</i> , 2018 , 18, 1620-1627	11.5	9
235	Ultrafast Electric Field Pulse Control of Giant Temperature Change in Ferroelectrics. <i>Physical Review Letters</i> , 2018 , 120, 055901	7.4	14
234	Ab Initio Simulation Explains the Enhancement of Catalytic Oxygen Evolution on CaMnO ₃ . <i>ACS Catalysis</i> , 2018 , 8, 2218-2224	13.1	17
233	Experimental and Theoretical Study of the Self-Initiation Reaction of Methyl Acrylate in Free-Radical Polymerization. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 532-539	3.9	16
232	Improper magnetic ferroelectricity of nearly pure electronic nature in helicoidal spiral CaMn ₇ O ₁₂ . <i>Physical Review B</i> , 2018 , 97,	3.3	8
231	First-principles studies of the local structure and relaxor behavior of Pb(Mg _{1/3} Nb _{2/3})O ₃ BbTiO ₃ -derived ferroelectric perovskite solid solutions. <i>Physical Review B</i> , 2018 , 97,	3.3	14
230	What Remains Unexplained about the Properties of Halide Perovskites?. <i>Advanced Materials</i> , 2018 , 30, e1800691	24	174
229	Chemical Pressure-Driven Enhancement of the Hydrogen Evolving Activity of NiP from Nonmetal Surface Doping Interpreted via Machine Learning. <i>Journal of the American Chemical Society</i> , 2018 , 140, 4678-4683	16.4	87
228	Design of Metal-Halide Inverse-Hybrid Perovskites. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 13872-13883	3.8	7
227	Enhancing ferroelectric photovoltaic effect by polar order engineering. <i>Science Advances</i> , 2018 , 4, eaat3428	14.8	88
226	On the Thermal Self-Initiation Reaction of n-Butyl Acrylate in Free-Radical Polymerization. <i>Processes</i> , 2018 , 6, 3	2.9	17
225	Wallpaper fermions and the nonsymmorphic Dirac insulator. <i>Science</i> , 2018 , 361, 246-251	33.3	73
224	Control of the Polarization of Ferroelectric Capacitors by the Concurrent Action of Light and Adsorbates. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 23968-23975	9.5	8
223	Ubiquitous Short-Range Distortion of Hybrid Perovskites and Hydrogen-Bonding Role: the MAPbCl ₃ Case. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 28265-28272	3.8	16

222	How Lattice and Charge Fluctuations Control Carrier Dynamics in Halide Perovskites. <i>Nano Letters</i> , 2018 , 18, 8041-8046	11.5	51
221	Doping of BiFeO ₃ : A comprehensive study on substitutional doping. <i>Physical Review B</i> , 2018 , 98,	3.3	36
220	Dirac-Weyl Semimetal: Coexistence of Dirac and Weyl Fermions in Polar Hexagonal ABC Crystals. <i>Physical Review Letters</i> , 2018 , 121, 106404	7.4	34
219	Ionic gating drives correlated insulator-metal transition. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, 9655-9657	11.5	2
218	Long-lived polarization memory in the electronic states of lead-halide perovskites from local structural dynamics. <i>Nature Communications</i> , 2018 , 9, 3531	17.4	21
217	Transition metal inverse-hybrid perovskites. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 14560-14565	13	9
216	Seeing the forest and the trees. <i>Nature Materials</i> , 2018 , 17, 657-658	27	5
215	Phonon Influence on Bulk Photovoltaic Effect in the Ferroelectric Semiconductor GeTe. <i>Physical Review Letters</i> , 2018 , 121, 017402	7.4	17
214	Giant Bulk Photovoltaic Effect in Vinylene-Linked Hybrid Heterocyclic Polymer. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 6500-6507	3.8	11
213	Large-area synthesis of high-quality monolayer 1T'-WTe flakes. <i>2D Materials</i> , 2017 , 4,	5.9	56
212	Influence of the Dimensionality and Organic Cation on Crystal and Electronic Structure of Organometallic Halide Perovskites. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 6569-6574	3.8	33
211	Large polarization gradients and temperature-stable responses in compositionally-graded ferroelectrics. <i>Nature Communications</i> , 2017 , 8, 14961	17.4	43
210	Reply to 'Reconsidering the Shockley-Queisser limit of a ferroelectric insulator device'. <i>Nature Photonics</i> , 2017 , 11, 330-330	33.9	1
209	Asymmetry in mechanical polarization switching. <i>Applied Physics Letters</i> , 2017 , 110, 222903	3.4	13
208	Slush-like polar structures in single-crystal relaxors. <i>Nature</i> , 2017 , 546, 391-395	50.4	128
207	Local Polar Fluctuations in Lead Halide Perovskite Crystals. <i>Physical Review Letters</i> , 2017 , 118, 136001	7.4	374
206	Frequency-dependent dielectric function of semiconductors with application to physisorption. <i>Physical Review B</i> , 2017 , 95,	3.3	18
205	Intermolecular Interactions in Hybrid Perovskites Understood From a Combined Density Functional Theory and Effective Hamiltonian Approach. <i>ACS Energy Letters</i> , 2017 , 2, 937-942	20.1	25

204	Adsorption of Benzene on the RuO ₂ (110) Surface. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 1585-1590	3.8	4
203	Active Role of Phosphorus in the Hydrogen Evolving Activity of Nickel Phosphide (0001) Surfaces. <i>ACS Catalysis</i> , 2017 , 7, 7718-7725	13.1	70
202	Adding to the Perovskite Universe: Inverse-Hybrid Perovskites. <i>ACS Energy Letters</i> , 2017 , 2, 2681-2685	20.1	20
201	Light-induced picosecond rotational disordering of the inorganic sublattice in hybrid perovskites. <i>Science Advances</i> , 2017 , 3, e1602388	14.3	109
200	Polarized emission in II-VI and perovskite colloidal quantum dots. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2017 , 50, 214001	1.3	2
199	Tuning the gap of lead-based halide perovskites by introducing superalkali species at the cationic sites of ABX ₃ -type structure. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 20619-20626	3.6	10
198	Synthesis and Physical Properties of Phase-Engineered Transition Metal Dichalcogenide Monolayer Heterostructures. <i>ACS Nano</i> , 2017 , 11, 8619-8627	16.7	34
197	Rashba Effect in a Single Colloidal CsPbBr ₃ Perovskite Nanocrystal Detected by Magneto-Optical Measurements. <i>Nano Letters</i> , 2017 , 17, 5020-5026	11.5	143
196	Getting a charge out of hybrid perovskites. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 7191-7193	11.5	9
195	Thin-film ferroelectric materials and their applications. <i>Nature Reviews Materials</i> , 2017 , 2,	73.3	350
194	A DFT study on the hydrogen desorption from the lithium borohydride and aluminohydride upon the addition of nanostructured carbon catalyzing agent. <i>International Journal of Hydrogen Energy</i> , 2017 , 42, 3019-3026	6.7	4
193	Structural and ferroelectric phase evolution in [KNbO ₃] _{1-x} [BaNi _{1/2} Nb _{1/2} O ₃] _x (x=0,0.1). <i>Physical Review B</i> , 2017 , 96,	3.3	20
192	Screened van der Waals correction to density functional theory for solids. <i>Physical Review Materials</i> , 2017 , 1,	3.2	18
191	Two-Dimensional Conjugated Covalent-Organic Frameworks as Quantum Anomalous Hall Topological Insulators. <i>Physical Review Letters</i> , 2016 , 116, 096601	7.4	65
190	Double Dirac Semimetals in Three Dimensions. <i>Physical Review Letters</i> , 2016 , 116, 186402	7.4	199
189	Stable Phosphorus-Enriched (0001) Surfaces of Nickel Phosphides. <i>Chemistry of Materials</i> , 2016 , 28, 5365-5372	5.3	33
188	Substantial optical dielectric enhancement by volume compression in LiAsSe ₂ . <i>Physical Review B</i> , 2016 , 93,	3.3	1
187	Enhancement of the Bulk Photovoltaic Effect in Topological Insulators. <i>Physical Review Letters</i> , 2016 , 116, 237402	7.4	34

186	Electron-beam-induced ferroelectric domain behavior in the transmission electron microscope: Toward deterministic domain patterning. <i>Physical Review B</i> , 2016 , 94,	3.3	19
185	Atomistic description for temperature-driven phase transitions in BaTiO ₃ . <i>Physical Review B</i> , 2016 , 94,	3.3	28
184	Improved pseudopotential transferability for magnetic and electronic properties of binary manganese oxides from DFT+U+J calculations. <i>Physical Review B</i> , 2016 , 94,	3.3	22
183	Communication: Accurate higher-order van der Waals coefficients between molecules from a model dynamic multipole polarizability. <i>Journal of Chemical Physics</i> , 2016 , 144, 031102	3.9	17
182	Valence Band Control of Metal Silicide Films via Stoichiometry. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 2573-8	6.4	6
181	Intrinsic ferroelectric switching from first principles. <i>Nature</i> , 2016 , 534, 360-3	50.4	101
180	Strain-Induced Ferroelectric Topological Insulator. <i>Nano Letters</i> , 2016 , 16, 1663-8	11.5	67
179	Surface Chemically Switchable Ultraviolet Luminescence from Interfacial Two-Dimensional Electron Gas. <i>Nano Letters</i> , 2016 , 16, 681-7	11.5	9
178	Photoferroelectric and Photopiezoelectric Properties of Organometal Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 1460-5	6.4	59
177	Hybrid Organic-Inorganic Perovskites on the Move. <i>Accounts of Chemical Research</i> , 2016 , 49, 573-81	24.3	176
176	Asymmetric Response of Ferroelastic Domain-Wall Motion under Applied Bias. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 2935-41	9.5	8
175	Theoretical Modeling of Tribochemical Reaction on Pt and Au Contacts: Mechanical Load and Catalysis. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 7529-35	9.5	14
174	Study of n-Butyl Acrylate Self-Initiation Reaction Experimentally and via Macroscopic Mechanistic Modeling. <i>Processes</i> , 2016 , 4, 15	2.9	13
173	Interplay between Cation and Charge Ordering in La _{1/3} Sr _{2/3} FeO ₃ Superlattices. <i>Advanced Electronic Materials</i> , 2016 , 2, 1500372	6.4	6
172	Origin and structure of polar domains in doped molecular crystals. <i>Nature Communications</i> , 2016 , 7, 13351	17.4	24
171	Shift current bulk photovoltaic effect in polar materials—Hybrid and oxide perovskites and beyond. <i>Npj Computational Materials</i> , 2016 , 2,	10.9	142
170	Substantial bulk photovoltaic effect enhancement via nanolayering. <i>Nature Communications</i> , 2016 , 7, 10419	17.4	51
169	Monolayer Single-Crystal 1T'-MoTe ₂ Grown by Chemical Vapor Deposition Exhibits Weak Antilocalization Effect. <i>Nano Letters</i> , 2016 , 16, 4297-304	11.5	167

168	High Chloride Doping Levels Stabilize the Perovskite Phase of Cesium Lead Iodide. <i>Nano Letters</i> , 2016 , 16, 3563-70	11.5	208
167	Direct Observation of Electron-Phonon Coupling and Slow Vibrational Relaxation in Organic-Inorganic Hybrid Perovskites. <i>Journal of the American Chemical Society</i> , 2016 , 138, 13798-13801	16.4	147
166	Design of New Complexes of Inorganic Salts Based on Lithium and Magnesium Hydroxides and Carbonates for Usage as Propellants and Flame Retardants. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 7764-7770	2.8	3
165	Assemblage of Superalkali Complexes with Ever Low-Ionization Potentials. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 6493-9	2.8	7
164	Power conversion efficiency exceeding the Shockley-Queisser limit in a ferroelectric insulator. <i>Nature Photonics</i> , 2016 , 10, 611-616	33.9	224
163	Ferroelectrically driven spatial carrier density modulation in graphene. <i>Nature Communications</i> , 2015 , 6, 6136	17.4	107
162	Dynamical screening of van der Waals interactions in nanostructured solids: Sublimation of fullerenes. <i>Journal of Chemical Physics</i> , 2015 , 142, 164302	3.9	14
161	First-principles calculation of the bulk photovoltaic effect in KNbO ₃ and (K,Ba)(Ni,Nb)O ₃ □	3.3	47
160	Polarization Dependence of Water Adsorption to CH ₃ NH ₃ PbI ₃ (001) Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 4371-8	6.4	93
159	Materials Design of Visible-Light Ferroelectric Photovoltaics from First Principles. <i>Ferroelectrics</i> , 2015 , 483, 1-12	0.6	27
158	Rashba Spin-Orbit Coupling Enhanced Carrier Lifetime in CH ₃ NH ₃ PbI ₃ □ <i>Nano Letters</i> , 2015 , 15, 7794-800	11.5	363
157	Are Mobilities in Hybrid Organic-Inorganic Halide Perovskites Actually "High"? <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 4754-7	6.4	167
156	Material Innovation in Advancing Organometal Halide Perovskite Functionality. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 4862-72	6.4	35
155	First-Principles Calculation of the Bulk Photovoltaic Effect in CH ₃ NH ₃ PbI ₃ and CH ₃ NH ₃ PbI(3-x)Cl(x). <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 31-7	6.4	155
154	Ferroelectric polarization reversal via successive ferroelastic transitions. <i>Nature Materials</i> , 2015 , 14, 79-86	16.7	175
153	Theory of Hydrogen Migration in Organic-Inorganic Halide Perovskites. <i>Angewandte Chemie</i> , 2015 , 127, 12614-12618	3.6	7
152	Designing Ferroelectric Field-Effect Transistors Based on the Polarization-Rotation Effect for Low Operating Voltage and Fast Switching. <i>Physical Review Applied</i> , 2015 , 4,	4.3	13
151	First-Principles Materials Design of High-Performing Bulk Photovoltaics with the LiNbO ₃ Structure. <i>Physical Review Applied</i> , 2015 , 4,	4.3	26

150	Controlling oxide surface dipole and reactivity with intrinsic nonstoichiometric epitaxial reconstructions. <i>Physical Review B</i> , 2015 , 92,	3-3	12
149	Dirac Line Nodes in Inversion-Symmetric Crystals. <i>Physical Review Letters</i> , 2015 , 115, 036806	7-4	534
148	Layered Topological Crystalline Insulators. <i>Physical Review Letters</i> , 2015 , 115, 086802	7-4	24
147	Modified Schottky emission to explain thickness dependence and slow depolarization in BaTiO ₃ nanowires. <i>Physical Review B</i> , 2015 , 91,	3-3	3
146	Electronic transition above room temperature in CaMn ₇ O ₁₂ films. <i>Applied Physics Letters</i> , 2015 , 107, 142901	3-4	8
145	Unusually Large Young's Moduli of Amino Acid Molecular Crystals. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 13566-70	16.4	54
144	Hybrid Organic-Inorganic Perovskites (HOIPs): Opportunities and Challenges. <i>Advanced Materials</i> , 2015 , 27, 5102-12	24	325
143	Ultrafast Terahertz Gating of the Polarization and Giant Nonlinear Optical Response in BiFeO ₃ Thin Films. <i>Advanced Materials</i> , 2015 , 27, 6371-5	24	34
142	Unusually Large Young's Moduli of Amino Acid Molecular Crystals. <i>Angewandte Chemie</i> , 2015 , 127, 13770-13774	16.4	112
141	Theory of hydrogen migration in organic-inorganic halide perovskites. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 12437-41	16.4	112
140	Novel materials solutions and simulations for nanoelectromechanical switches 2015 ,		5
139	Theoretical Study of Intermolecular Chain Transfer to Polymer Reactions of Alkyl Acrylates. <i>Industrial & Engineering Chemistry Research</i> , 2015 , 54, 4148-4165	3-9	14
138	Synergistic oxygen evolving activity of a TiO ₂ -rich reconstructed SrTiO ₃ (001) surface. <i>Journal of the American Chemical Society</i> , 2015 , 137, 2939-47	16.4	55
137	Ferroelectric Domain Wall Induced Band Gap Reduction and Charge Separation in Organometal Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 693-9	6-4	258
136	Physical adsorption: theory of van der Waals interactions between particles and clean surfaces. <i>Physical Review Letters</i> , 2014 , 112, 106101	7-4	44
135	Bulk Dirac points in distorted spinels. <i>Physical Review Letters</i> , 2014 , 112, 036403	7-4	123
134	Strong reciprocal interaction between polarization and surface stoichiometry in oxide ferroelectrics. <i>Nano Letters</i> , 2014 , 14, 6711-7	11-5	29
133	Semiconducting ferroelectric photovoltaics through Zn ²⁺ doping into KNbO ₃ and polarization rotation. <i>Physical Review B</i> , 2014 , 89,	3-3	38

132	Backbiting and Scission reactions in free-radical polymerization of methyl acrylate. <i>International Journal of Quantum Chemistry</i> , 2014 , 114, 345-360	2.1	31
131	Semiconducting ferroelectric perovskites with intermediate bands via B-site Bi ⁵⁺ doping. <i>Physical Review B</i> , 2014 , 90,	3.3	19
130	Computational Studies of Lead-based Relaxor Ferroelectrics. <i>Ferroelectrics</i> , 2014 , 469, 1-13	0.6	7
129	Theoretical Model of Oxidative Adsorption of Water on a Highly Reduced Reconstructed Oxide Surface. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 3408-14	6.4	24
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