Andrew M Rappe

List of Publications by Year
in descending order

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Version: 2024-02-01

303 papers	27,513 citations	6606 79 h-index	6294 158 g-index
307 all docs	307 docs citations	307 times ranked	25090 citing authors

#	Article	IF	Citations
1	Mechanochemical Molecular Migration on Graphene. Journal of the American Chemical Society, 2022, 144, 7181-7188.	6.6	8
2	Structure, Diffusion, and Stability of Lithium Salts in Aprotic Dimethyl Sulfoxide and Acetonitrile Electrolytes. Journal of Physical Chemistry C, 2022, 126, 10266-10272.	1.5	7
3	Developing a force field for the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ba</mml:mi><mml:mrow><mml:mn>1</mml:mn> ferroelectric alloy: Prediction of a ferroelectric superlattice structure. Physical Review B, 2022, 105, .	3.7	5
4	A charge transfer framework that describes supramolecular interactions governing structure and properties of 2D perovskites. Nature Communications, 2022, 13, .	5.8	16
5	Comprehensive defect suppression in perovskite nanocrystals for high-efficiency light-emitting diodes. Nature Photonics, 2021, 15, 148-155.	15.6	590
6	Metal cation s lone-pairs increase octahedral tilting instabilities in halide perovskites. Materials Advances, 2021, 2, 4610-4616.	2.6	20
7	Large Bulk Piezophotovoltaic Effect of Monolayer 2H-MoS₂. Journal of Physical Chemistry Letters, 2021, 12, 1244-1249.	2.1	37
8	Hydrogen freedom linked to perovskite efficiency. Nature Materials, 2021, 20, 914-915.	13.3	1
9	Phonon-Assisted Ballistic Current from First-Principles Calculations. Physical Review Letters, 2021, 126, 177403.	2.9	32
10	Widespread Negative Longitudinal Piezoelectric Responses in Ferroelectric Crystals with Layered Structures. Physical Review Letters, 2021, 126, 217601.	2.9	42
11	Strongly Anharmonic Octahedral Tilting in Two-Dimensional Hybrid Halide Perovskites. ACS Nano, 2021, 15, 10153-10162.	7.3	59
12	The Significance of Polarons and Dynamic Disorder in Halide Perovskites. ACS Energy Letters, 2021, 6, 2162-2173.	8.8	74
13	Oxygen-Initiated Free-Radical Polymerization of Alkyl Acrylates at High Temperatures. Macromolecules, 2021, 54, 7925-7930.	2.2	3
14	Mechanistic Insights into CO₂ Electroreduction on Ni₂P: Understanding Its Selectivity toward Multicarbon Products. ACS Catalysis, 2021, 11, 11706-11715.	5.5	20
15	Stromataxic Stabilization of a Metastable Layered ScFeO₃ Polymorph. Chemistry of Materials, 2021, 33, 7423-7431.	3.2	6
16	Mechanistic Study of the Liâ€“Air Battery with a Co3O4 Cathode and Dimethyl Sulfoxide Electrolyte. Journal of Physical Chemistry C, 2021, 125, 21873-21881.	1.5	9
17	Intrinsic Fermi-surface contribution to the bulk photovoltaic effect. Physical Review Research, 2021, 3, .	1.3	23
18	Bulk photovoltaic effect in hexagonal LuMnO3 single crystals. Physical Review B, 2021, 104, .	1.1	7

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19	First-principles calculation of ballistic current from electron-hole interaction. Physical Review B, 2021, 104, .	1.1	8
20	Epitaxial TiO x Surface in Ferroelectric BaTiO 3 : Native Structure and Dynamic Patterning at the Atomic Scale. Advanced Functional Materials, 2020, 30, 1902549.	7.8	15
21	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. Journal of Chemical Theory and Computation, 2020, 16, 835-846.	2.3	8
22	Experimental and Mechanistic Modeling Study of Self-Initiated High-Temperature Polymerization of Ethyl Acrylate. Industrial & Engineering Chemistry Research, 2020, 59, 2621-2630.	1.8	12
23	Optical signatures of multifold fermions in the chiral topological semimetal CoSi. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 27104-27110.	3.3	37
24	Impact of Hierarchical Nanoporous Architectures on Sodium Storage in Antimony-Based Sodium-Ion Battery Anodes. ACS Applied Energy Materials, 2020, 3, 11231-11241.	2.5	11
25	Ferroelectric Switching of Pure Spin Polarization in Two-Dimensional Electron Gas. Nano Letters, 2020, 20, 7230-7236.	4.5	2
26	Shift photovoltaic current and magnetically induced bulk photocurrent in piezoelectric sillenite crystals. Physical Review B, 2020, 102, .	1.1	18
27	Kinetically Stable Oxide Overlayers on Mo₃P Nanoparticles Enabling Lithiumâ€“Air Batteries with Low Overpotentials and Long Cycle Life. Advanced Materials, 2020, 32, e2004028.	11.1	42
28	General Approach for Reducing Continuous Translational Symmetry Errors in Finite Difference Real-Space Calculations. Journal of Chemical Theory and Computation, 2020, 16, 4327-4336.	2.3	1
29	Unraveling the Elastic Properties of (Quasi)Two-Dimensional Hybrid Perovskites: A Joint Experimental and Theoretical Study. ACS Applied Materials & Interfaces, 2020, 12, 17881-17892.	4.0	21
30	Ideal near-Dirac triple-point semimetal in III-V semiconductor alloys. Physical Review B, 2020, 101, .	1.1	7
31	Origin of the anomalous Pb-Br bond dynamics in formamidinium lead bromide perovskites. Physical Review B, 2020, 101, .	1.1	14
32	Shift-current bulk photovoltaic effect influenced by quasiparticle and exciton. Physical Review B, 2020, 101, .	1.1	37
33	Large-area epitaxial growth of curvature-stabilized ABC trilayer graphene. Nature Communications, 2020, 11, 546.	5.8	47
34	Lattice mode symmetry analysis of the orthorhombic phase of methylammonium lead iodide using polarized Raman. Physical Review Materials, 2020, 4, .	0.9	20
35	Elucidating the atomistic origin of anharmonicity in tetragonal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>CH</mml:mi><mml:mn>3</mml:mn></ with Raman scattering. Physical Review Materials, 2020, 4, .	0.9	34
36	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	1.3	236

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37	Upper limit on shift current generation in extended systems. Physical Review B, 2019, 100, .	1.1	23
38	Spatially dispersive circular photogalvanic effect in a Weyl semimetal. Nature Materials, 2019, 18, 955-962.	13.3	99
39	Breakdown of the Static Picture of Defect Energetics in Halide Perovskites: The Case of the Br Vacancy in CsPbBr₃. Journal of Physical Chemistry Letters, 2019, 10, 4490-4498.	2.1	52
40	Topological Semimetals from First Principles. Annual Review of Materials Research, 2019, 49, 153-183.	4.3	154
41	Method of Moments Applied to Most-Likely High-Temperature Free-Radical Polymerization Reactions. Processes, 2019, 7, 656.	1.3	10
42	Surface Pyroelectricity in Cubic SrTiO₃. Advanced Materials, 2019, 31, e1904733.	11.1	54
43	Mechanochemical Effects of Adsorbates at Nanoelectromechanical Switch Contacts. ACS Applied Materials & Interfaces, 2019, 11, 39238-39247.	4.0	6
44	Terahertz fieldâ€“induced ferroelectricity in quantum paraelectric SrTiO ₃. Science, 2019, 364, 1079-1082.	6.0	282
45	Kinetic control of tunable multi-state switching in ferroelectric thin films. Nature Communications, 2019, 10, 1282.	5.8	47
46	Water in hybrid perovskites: Bulk MAPbI3 degradation via super-hydrous state. APL Materials, 2019, 7, .	2.2	42
47	Epitaxial Strain Control of Relaxor Ferroelectric Phase Evolution. Advanced Materials, 2019, 31, e1901060.	11.1	29
48	Bioferroelectric Properties of Glycine Crystals. Journal of Physical Chemistry Letters, 2019, 10, 1319-1324.	2.1	32
49	Theoretical Insights Into Thermal Self-Initiation Reactions of Acrylates. , 2019, , 99-134.		1
50	Theoretical Insights Into Chain Transfer Reactions of Acrylates. , 2019, , 135-193.		3
51	Ferroelectric barium titanate derivatives containing Mo and Mg for transparent photovoltaic applications. Journal of Applied Physics, 2019, 126, .	1.1	7
52	Sr-induced dipole scatter in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ba</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:mrow></mml:math> : Insights from a transferable-bond valence-based interatomic potential. Physical Review B, 2019, 100, .	1.1	18
53	In Situ Bottom-up Synthesis of Porphyrin-Based Covalent Organic Frameworks. Journal of the American Chemical Society, 2019, 141, 19560-19564.	6.6	55
54	Mix and Match: Organic and Inorganic Ions in the Perovskite Lattice. Advanced Materials, 2019, 31, e1802697.	11.1	37

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55	Automatic Prediction of Surface Phase Diagrams Using Ab Initio Grand Canonical Monte Carlo. Journal of Physical Chemistry C, 2019, 123, 2321-2328.	1.5	45
56	Effect of wavefunction delocalization on shift current generation. Journal of Physics Condensed Matter, 2019, 31, 084002.	0.7	9
57	Big data approach for effective ionic radii. Computer Physics Communications, 2019, 237, 238-243.	3.0	10
58	Spin-orbit enhanced carrier lifetimes in noncentrosymmetric semiconductors. Journal of Physics and Chemistry of Solids, 2019, 128, 225-230.	1.9	1
59	Crystalline Bilayer Graphene with Preferential Stacking from Niâ€“Cu Gradient Alloy. ACS Nano, 2018, 12, 2275-2282.	7.3	43
60	Molecule-Adsorbed Topological Insulator and Metal Surfaces: A Comparative First-Principles Study. Chemistry of Materials, 2018, 30, 1849-1855.	3.2	10
61	Climbing the Volcano of Electrocatalytic Activity while Avoiding Catalyst Corrosion: Ni₃P, a Hydrogen Evolution Electrocatalyst Stable in Both Acid and Alkali. ACS Catalysis, 2018, 8, 4408-4419.	5.5	178
62	Hybrid functional pseudopotentials. Physical Review B, 2018, 97, .	1.1	32
63	Mixed Valence Perovskite Cs₂Au₂I₆: A Potential Material for Thinâ€Film Pbâ€Free Photovoltaic Cells with Ultrahigh Efficiency. Advanced Materials, 2018, 30, e1707001.	11.1	79
64	Anion Exchange in IIâ€“VI Semiconducting Nanostructures via Atomic Templating. Nano Letters, 2018, 18, 1620-1627.	4.5	11
65	Ultrafast Electric Field Pulse Control of Giant Temperature Change in Ferroelectrics. Physical Review Letters, 2018, 120, 055901.	2.9	21
66	Ab Initio Simulation Explains the Enhancement of Catalytic Oxygen Evolution on CaMnO₃. ACS Catalysis, 2018, 8, 2218-2224.	5.5	30
67	Experimental and Theoretical Study of the Self-Initiation Reaction of Methyl Acrylate in Free-Radical Polymerization. Industrial & Engineering Chemistry Research, 2018, 57, 532-539.	1.8	23
68	Improper magnetic ferroelectricity of nearly pure electronic nature in helicoidal spiral <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">CaMn</mml:mi><mml:mn>7</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mn>12</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2018, 97, .	1.1	11
69	First-principles studies of the local structure and relaxor behavior of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mi>Pb</mml:mi><mml:mi mathvariant="normal">O</mml:mi. Physical Review B, 2018, 97, .	1.1	17
70	What Remains Unexplained about the Properties of Halide Perovskites?. Advanced Materials, 2018, 30, e1800691.	11.1	231
71	Chemical Pressure-Driven Enhancement of the Hydrogen Evolving Activity of Ni₂P from Nonmetal Surface Doping Interpreted via Machine Learning. Journal of the American Chemical Society, 2018, 140, 4678-4683.	6.6	145
72	Design of Metal-Halide Inverse-Hybrid Perovskites. Journal of Physical Chemistry C, 2018, 122, 13872-13883.	1.5	9

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73	Ubiquitous Short-Range Distortion of Hybrid Perovskites and Hydrogen-Bonding Role: the MAPbCl₃ Case. Journal of Physical Chemistry C, 2018, 122, 28265-28272.	1.5	21
74	How Lattice and Charge Fluctuations Control Carrier Dynamics in Halide Perovskites. Nano Letters, 2018, 18, 8041-8046.	4.5	97
75	Doping of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi></mml:mi></mml:math> : A comprehensive study on substitutional doping. Physical Review B, 2018, 98, .	3.7	50
76	Dirac-Weyl Semimetal: Coexistence of Dirac and Weyl Fermions in Polar Hexagonal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>A</mml:mi><mml:mi>B</mml:mi><mml:mi>C</mml:mi></mml:math> Crystals. Physical Review Letters, 2018, 121, 106404.	2.9	50
77	Ionic gating drives correlated insulatorâ€“metal transition. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 9655-9657.	3.3	2
78	Long-lived polarization memory in the electronic states of lead-halide perovskites from local structural dynamics. Nature Communications, 2018, 9, 3531.	5.8	29
79	Transition metal inverse-hybrid perovskites. Journal of Materials Chemistry A, 2018, 6, 14560-14565.	5.2	11
80	Seeing the forest and the trees. Nature Materials, 2018, 17, 657-658.	13.3	5
81	Phonon Influence on Bulk Photovoltaic Effect in the Ferroelectric Semiconductor GeTe. Physical Review Letters, 2018, 121, 017402.	2.9	30
82	Enhancing ferroelectric photovoltaic effect by polar order engineering. Science Advances, 2018, 4, eaat3438.	4.7	152
83	On the Thermal Self-Initiation Reaction of n-Butyl Acrylate in Free-Radical Polymerization. Processes, 2018, 6, 3.	1.3	24
84	Wallpaper fermions and the nonsymmorphic Dirac insulator. Science, 2018, 361, 246-251.	6.0	125
85	Control of the Polarization of Ferroelectric Capacitors by the Concurrent Action of Light and Adsorbates. ACS Applied Materials & Interfaces, 2018, 10, 23968-23975.	4.0	10
86	Giant Bulk Photovoltaic Effect in Vinylene-Linked Hybrid Heterocyclic Polymer. Journal of Physical Chemistry C, 2017, 121, 6500-6507.	1.5	15
87	Large-area synthesis of high-quality monolayer 1Tâ€™-WTe ₂ flakes. 2D Materials, 2017, 4, 021008.	2.0	81
88	Influence of the Dimensionality and Organic Cation on Crystal and Electronic Structure of Organometallic Halide Perovskites. Journal of Physical Chemistry C, 2017, 121, 6569-6574.	1.5	47
89	Large polarization gradients and temperature-stable responses in compositionally-graded ferroelectrics. Nature Communications, 2017, 8, 14961.	5.8	60
90	Reply to 'Reconsidering the Shockleyâ€“Queisser limit of a ferroelectric insulator device'. Nature Photonics, 2017, 11, 330-330.	15.6	2

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91	Asymmetry in mechanical polarization switching. Applied Physics Letters, 2017, 110, .	1.5	20
92	Slush-like polar structures in single-crystal relaxors. Nature, 2017, 546, 391-395.	13.7	201
93	Local Polar Fluctuations in Lead Halide Perovskite Crystals. Physical Review Letters, 2017, 118, 136001.	2.9	489
94	Frequency-dependent dielectric function of semiconductors with application to physisorption. Physical Review B, 2017, 95, .	1.1	25
95	Intermolecular Interactions in Hybrid Perovskites Understood from a Combined Density Functional Theory and Effective Hamiltonian Approach. ACS Energy Letters, 2017, 2, 937-942.	8.8	28
96	Adsorption of Benzene on the RuO₂(110) Surface. Journal of Physical Chemistry C, 2017, 121, 1585-1590.	1.5	5
97	Active Role of Phosphorus in the Hydrogen Evolving Activity of Nickel Phosphide (0001) Surfaces. ACS Catalysis, 2017, 7, 7718-7725.	5.5	104
98	Adding to the Perovskite Universe: Inverse-Hybrid Perovskites. ACS Energy Letters, 2017, 2, 2681-2685.	8.8	30
99	Light-induced picosecond rotational disordering of the inorganic sublattice in hybrid perovskites. Science Advances, 2017, 3, e1602388.	4.7	149
100	Polarized emission in IIâ€“VI and perovskite colloidal quantum dots. Journal of Physics B: Atomic, Molecular and Optical Physics, 2017, 50, 214001.	0.6	4
101	Tuning the gap of lead-based halide perovskites by introducing superalkali species at the cationic sites of ABX₃-type structure. Physical Chemistry Chemical Physics, 2017, 19, 20619-20626.	1.3	14
102	Synthesis and Physical Properties of Phase-Engineered Transition Metal Dichalcogenide Monolayer Heterostructures. ACS Nano, 2017, 11, 8619-8627.	7.3	42
103	Rashba Effect in a Single Colloidal CsPbBr₃ Perovskite Nanocrystal Detected by Magneto-Optical Measurements. Nano Letters, 2017, 17, 5020-5026.	4.5	180
104	Getting a charge out of hybrid perovskites. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 7191-7193.	3.3	12
105	Thin-film ferroelectric materials and their applications. Nature Reviews Materials, 2017, 2, .	23.3	590
106	A DFT study on the hydrogen desorption from the lithium borohydride and aluminohydride upon the addition of nanostructured carbon catalyzing agent. International Journal of Hydrogen Energy, 2017, 42, 3019-3026.	3.8	4
107	Structural and ferroelectric phase evolution in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mo>[</mml:mo> Physical Review B, 2017, 96, .	1.1	28
108	Screened van der Waals correction to density functional theory for solids. Physical Review Materials, 2017, 1, .	0.9	19

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109	Study of n-Butyl Acrylate Self-Initiation Reaction Experimentally and via Macroscopic Mechanistic Modeling. Processes, 2016, 4, 15.	1.3	16
110	Interplay between Cation and Charge Ordering in La_{1/3}Sr_{2/3}FeO₃ Superlattices. Advanced Electronic Materials, 2016, 2, 1500372.	2.6	8
111	Origin and structure of polar domains in doped molecular crystals. Nature Communications, 2016, 7, 13351.	5.8	36
112	Shift current bulk photovoltaic effect in polar materialsâ€"hybrid and oxide perovskites and beyond. Npj Computational Materials, 2016, 2, .	3.5	246
113	Substantial bulk photovoltaic effect enhancement via nanolayering. Nature Communications, 2016, 7, 10419.	5.8	62
114	Monolayer Single-Crystal 1Tâ€²-MoTe₂ Grown by Chemical Vapor Deposition Exhibits Weak Antilocalization Effect. Nano Letters, 2016, 16, 4297-4304.	4.5	205
115	High Chloride Doping Levels Stabilize the Perovskite Phase of Cesium Lead Iodide. Nano Letters, 2016, 16, 3563-3570.	4.5	247
116	Direct Observation of Electronâ€"Phonon Coupling and Slow Vibrational Relaxation in Organicâ€"Inorganic Hybrid Perovskites. Journal of the American Chemical Society, 2016, 138, 13798-13801.	6.6	196
117	Design of New Complexes of Inorganic Salts Based on Lithium and Magnesium Hydroxides and Carbonates for Usage as Propellants and Flame Retardants. Journal of Physical Chemistry A, 2016, 120, 7764-7770.	1.1	5
118	Assemblage of Superalkali Complexes with Ever Low-Ionization Potentials. Journal of Physical Chemistry A, 2016, 120, 6493-6499.	1.1	8
119	Power conversion efficiency exceeding the Shockleyâ€"Queisser limit in a ferroelectric insulator. Nature Photonics, 2016, 10, 611-616.	15.6	335
120	Two-Dimensionalï€-Conjugated Covalent-Organic Frameworks as Quantum Anomalous Hall Topological Insulators. Physical Review Letters, 2016, 116, 096601.	2.9	75
121	Double Dirac Semimetals in Three Dimensions. Physical Review Letters, 2016, 116, 186402.	2.9	273
122	Stable Phosphorus-Enriched (0001) Surfaces of Nickel Phosphides. Chemistry of Materials, 2016, 28, 5365-5372.	3.2	48
123	Substantial optical dielectric enhancement by volume compression inLiAsSe2. Physical Review B, 2016, 93, .	1.1	1
124	Enhancement of the Bulk Photovoltaic Effect in Topological Insulators. Physical Review Letters, 2016, 116, 237402.	2.9	61
125	Electron-beam-induced ferroelectric domain behavior in the transmission electron microscope: Toward deterministic domain patterning. Physical Review B, 2016, 94, .	1.1	26
126	Atomistic description for temperature-driven phase transitions in <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></m Physical Review B, 2016, 94, .	1.1	52

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127	Improved pseudopotential transferability for magnetic and electronic properties of binary manganese oxides from <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi><mml:mo>+</mml:mo><mml:mi>J</mml:mi></mml calculations. Physical Review B, 2016, 94, .	1.1	30
128	Communication: Accurate higher-order van der Waals coefficients between molecules from a model dynamic multipole polarizability. Journal of Chemical Physics, 2016, 144, 031102.	1.2	22
129	Valence Band Control of Metal Silicide Films via Stoichiometry. Journal of Physical Chemistry Letters, 2016, 7, 2573-2578.	2.1	6
130	Intrinsic ferroelectric switching from first principles. Nature, 2016, 534, 360-363.	13.7	151
131	Strain-Induced Ferroelectric Topological Insulator. Nano Letters, 2016, 16, 1663-1668.	4.5	82
132	Surface Chemically Switchable Ultraviolet Luminescence from Interfacial Two-Dimensional Electron Gas. Nano Letters, 2016, 16, 681-687.	4.5	11
133	Photoferroelectric and Photopiezoelectric Properties of Organometal Halide Perovskites. Journal of Physical Chemistry Letters, 2016, 7, 1460-1465.	2.1	73
134	Hybrid Organicâ€“Inorganic Perovskites on the Move. Accounts of Chemical Research, 2016, 49, 573-581.	7.6	227
135	Asymmetric Response of Ferroelastic Domain-Wall Motion under Applied Bias. ACS Applied Materials & Interfaces, 2016, 8, 2935-2941.	4.0	11
136	Theoretical Modeling of Tribochemical Reaction on Pt and Au Contacts: Mechanical Load and Catalysis. ACS Applied Materials & Interfaces, 2016, 8, 7529-7535.	4.0	23
137	Theory of Hydrogen Migration in Organicâ€“Inorganic Halide Perovskites. Angewandte Chemie, 2015, 127, 12614-12618.	1.6	8
138	Designing Ferroelectric Field-Effect Transistors Based on the Polarization-Rotation Effect for Low Operating Voltage and Fast Switching. Physical Review Applied, 2015, 4, .	1.5	15
139	First-Principles Materials Design of High-Performing Bulk Photovoltaics with the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Li</mml:mi><mml:mi>Nb</mml:mi><mml:msub><mml:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml Physical Review Applied, 2015, 4, .	1.5	30
140	Controlling oxide surface dipole and reactivity with intrinsic nonstoichiometric epitaxial reconstructions. Physical Review B, 2015, 92, .	1.1	14
141	Dirac Line Nodes in Inversion-Symmetric Crystals. Physical Review Letters, 2015, 115, 036806.	2.9	674
142	Layered Topological Crystalline Insulators. Physical Review Letters, 2015, 115, 086802.	2.9	28
143	Modified Schottky emission to explain thickness dependence and slow depolarization in<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><mml:msub> Physical Review B, 2015, 91, .	1.1	3
144	Electronic transition above room temperature in CaMn7O12 films. Applied Physics Letters, 2015, 107, 142901.	1.5	9

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145	Unusually Large Youngâ€™s Moduli of Amino Acid Molecular Crystals. Angewandte Chemie - International Edition, 2015, 54, 13566-13570.	7.2	83
146	Hybrid Organicâ€“Inorganic Perovskites (HOIPs): Opportunities and Challenges. Advanced Materials, 2015, 27, 5102-5112.	11.1	372
147	Ultrafast Terahertz Gating of the Polarization and Giant Nonlinear Optical Response in BiFeO₃ Thin Films. Advanced Materials, 2015, 27, 6371-6375.	11.1	47
148	Theory of Hydrogen Migration in Organicâ€“Inorganic Halide Perovskites. Angewandte Chemie - International Edition, 2015, 54, 12437-12441.	7.2	134
149	Novel materials solutions and simulations for nanoelectromechanical switches. , 2015, , .		5
150	Theoretical Study of Intermolecular Chain Transfer to Polymer Reactions of Alkyl Acrylates. Industrial & Engineering Chemistry Research, 2015, 54, 4148-4165.	1.8	20
151	Synergistic Oxygen Evolving Activity of a TiO₂-Rich Reconstructed SrTiO₃(001) Surface. Journal of the American Chemical Society, 2015, 137, 2939-2947.	6.6	58
152	Ferroelectric Domain Wall Induced Band Gap Reduction and Charge Separation in Organometal Halide Perovskites. Journal of Physical Chemistry Letters, 2015, 6, 693-699.	2.1	293
153	Ferroelectrically driven spatial carrier density modulation in graphene. Nature Communications, 2015, 6, 6136.	5.8	142
154	Dynamical screening of van der Waals interactions in nanostructured solids: Sublimation of fullerenes. Journal of Chemical Physics, 2015, 142, 164302.	1.2	15
155	First-principles calculation of the bulk photovoltaic effect in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">KNbO</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:math>and (K,Ba)(Ni,Nb)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn><mml:mo>â^’</mml:mo><mml:mi>δ</mml:mi></	1.1	53
156	Polarization Dependence of Water Adsorption to CH₃NH₃PbI₃ (001) Surfaces. Journal of Physical Chemistry Letters, 2015, 6, 4371-4378.	2.1	111
157	Materials Design of Visible-Light Ferroelectric Photovoltaics from First Principles. Ferroelectrics, 2015, 483, 1-12.	0.3	27
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