Andrew M Rappe

List of Publications by Year
in descending order

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	Optimized pseudopotentials. Physical Review B, 1990, 41, 1227-1230.	1.1	2,139
2	Dirac Semimetal in Three Dimensions. Physical Review Letters, 2012, 108, 140405.	2.9	1,388
3	Perovskite oxides for visible-light-absorbing ferroelectric and photovoltaic materials. Nature, 2013, 503, 509-512.	13.7	1,110
4	Donor and acceptor modes in photonic band structure. Physical Review Letters, 1991, 67, 3380-3383.	2.9	786
5	Dirac Line Nodes in Inversion-Symmetric Crystals. Physical Review Letters, 2015, 115, 036806.	2.9	674
6	Thin-film ferroelectric materials and their applications. Nature Reviews Materials, 2017, 2, .	23.3	590
7	Comprehensive defect suppression in perovskite nanocrystals for high-efficiency light-emitting diodes. Nature Photonics, 2021, 15, 148-155.	15.6	590
8	Local Polar Fluctuations in Lead Halide Perovskite Crystals. Physical Review Letters, 2017, 118, 136001.	2.9	489
9	Rashba Spinâ€“Orbit Coupling Enhanced Carrier Lifetime in CH₃NH₃PbI₃. Nano Letters, 2015, 15, 7794-7800.	4.5	438
10	First Principles Calculation of the Shift Current Photovoltaic Effect in Ferroelectrics. Physical Review Letters, 2012, 109, 116601.	2.9	414
11	Accurate theoretical analysis of photonic band-gap materials. Physical Review B, 1993, 48, 8434-8437.	1.1	402
12	Hybrid Organicâ€“Inorganic Perovskites (HOIPs): Opportunities and Challenges. Advanced Materials, 2015, 27, 5102-5112.	11.1	372
13	Ferroelectric Phase Transition in Individual Single-Crystalline BaTiO3 Nanowires. Nano Letters, 2006, 6, 735-739.	4.5	371
14	Electromagnetic Bloch waves at the surface of a photonic crystal. Physical Review B, 1991, 44, 10961-10964.	1.1	345
15	Stabilization of Monodomain Polarization in UltrathinPbTiO3Films. Physical Review Letters, 2006, 96, 127601.	2.9	344
16	Measurement of photonic band structure in a two-dimensional periodic dielectric array. Physical Review Letters, 1992, 68, 2023-2026.	2.9	341
17	Nucleation and growth mechanism of ferroelectric domain-wall motion. Nature, 2007, 449, 881-884.	13.7	340
18	Existence of a photonic band gap in two dimensions. Applied Physics Letters, 1992, 61, 495-497.	1.5	338

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19	Power conversion efficiency exceeding the Shockleyâ€“Queisser limit in a ferroelectric insulator. Nature Photonics, 2016, 10, 611-616.	15.6	335
20	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
21	Terahertz fieldâ€“induced ferroelectricity in quantum paraelectric SrTiO ₃. Science, 2019, 364, 1079-1082.	6.0	282
22	Double Dirac Semimetals in Three Dimensions. Physical Review Letters, 2016, 116, 186402.	2.9	273
23	Ferroelectricity in ultrathin perovskite films. Physical Review B, 2005, 72, .	1.1	249
24	High Chloride Doping Levels Stabilize the Perovskite Phase of Cesium Lead Iodide. Nano Letters, 2016, 16, 3563-3570.	4.5	247
25	Shift current bulk photovoltaic effect in polar materialsâ€”hybrid and oxide perovskites and beyond. Npj Computational Materials, 2016, 2, .	3.5	246
26	Reversible Chemical Switching of a Ferroelectric Film. Physical Review Letters, 2009, 102, 047601.	2.9	239
27	Relationship between local structure and phase transitions of a disordered solid solution. Nature, 2002, 419, 909-911.	13.7	238
28	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	1.3	236
29	What Remains Unexplained about the Properties of Halide Perovskites?. Advanced Materials, 2018, 30, e1800691.	11.1	231
30	Structure and energetics of alkanethiol adsorption on the Au(111) surface. Journal of Chemical Physics, 2002, 117, 825-833.	1.2	227
31	Hybrid Organicâ€“Inorganic Perovskites on the Move. Accounts of Chemical Research, 2016, 49, 573-581.	7.6	227
32	Ferroelectric polarization reversal via successive ferroelastic transitions. Nature Materials, 2015, 14, 79-86.	13.3	216
33	Designed nonlocal pseudopotentials for enhanced transferability. Physical Review B, 1999, 59, 12471-12478.	1.1	213
34	First-Principles Calculation of the Bulk Photovoltaic Effect in Bismuth Ferrite. Physical Review Letters, 2012, 109, 236601.	2.9	211
35	Monolayer Single-Crystal 1Tâ€²-MoTe₂ Grown by Chemical Vapor Deposition Exhibits Weak Antilocalization Effect. Nano Letters, 2016, 16, 4297-4304.	4.5	205
36	Slush-like polar structures in single-crystal relaxors. Nature, 2017, 546, 391-395.	13.7	201

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37	Predicting morphotropic phase boundary locations and transition temperatures in Pb- and Bi-based perovskite solid solutions from crystal chemical data and first-principles calculations. Journal of Applied Physics, 2005, 98, 094111.	1.1	199
38	Are Mobilities in Hybrid Organicâ€“Inorganic Halide Perovskites Actually â€œHighâ€?. Journal of Physical Chemistry Letters, 2015, 6, 4754-4757.	2.1	197
39	Direct in situ determination of the polarization dependence of physisorption on ferroelectric surfaces. Nature Materials, 2008, 7, 473-477.	13.3	196
40	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
41	Rashba Effect in a Single Colloidal CsPbBr₃ Perovskite Nanocrystal Detected by Magneto-Optical Measurements. Nano Letters, 2017, 17, 5020-5026.	4.5	180
42	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
43	First-Principles Calculation of the Bulk Photovoltaic Effect in CH₃NH₃PbI₃ and CH₃NH₃PbI_{3â€“x}Cl_x. Journal of Physical Chemistry Letters, 2015, 6, 31-37.	2.1	177
44	Continuous Growth of Hexagonal Graphene and Boron Nitride In-Plane Heterostructures by Atmospheric Pressure Chemical Vapor Deposition. ACS Nano, 2013, 7, 10129-10138.	7.3	170
45	New Highly Polar Semiconductor Ferroelectrics throughd⁸Cation-O Vacancy Substitution into PbTiO₃: A Theoretical Study. Journal of the American Chemical Society, 2008, 130, 17409-17412.	6.6	167
46	Photonic bound states in periodic dielectric materials. Physical Review B, 1991, 44, 13772-13774.	1.1	164
47	Growth Mechanism of Hexagonal-Shape Graphene Flakes with Zigzag Edges. ACS Nano, 2011, 5, 9154-9160.	7.3	154
48	Topological Semimetals from First Principles. Annual Review of Materials Research, 2019, 49, 153-183.	4.3	154
49	Enhancing ferroelectric photovoltaic effect by polar order engineering. Science Advances, 2018, 4, eaat3438.	4.7	152
50	Intrinsic ferroelectric switching from first principles. Nature, 2016, 534, 360-363.	13.7	151
51	Ultrafast Photovoltaic Response in Ferroelectric Nanolayers. Physical Review Letters, 2012, 108, 087601.	2.9	150
52	Bulk Dirac Points in Distorted Spinels. Physical Review Letters, 2014, 112, 036403.	2.9	150
53	Light-induced picosecond rotational disordering of the inorganic sublattice in hybrid perovskites. Science Advances, 2017, 3, e1602388.	4.7	149
54	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

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55	Ferroelectrically driven spatial carrier density modulation in graphene. Nature Communications, 2015, 6, 6136.	5.8	142
56	Virtual-crystal approximation that works: Locating a compositional phase boundary inPb(Zr1â^'xTix)O3. Physical Review B, 2000, 62, R743-R746.	1.1	136
57	Theory of Hydrogen Migration in Organicâ€“Inorganic Halide Perovskites. Angewandte Chemie - International Edition, 2015, 54, 12437-12441.	7.2	134
58	Observation of surface photons on periodic dielectric arrays. Optics Letters, 1993, 18, 528.	1.7	132
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73	How Lattice and Charge Fluctuations Control Carrier Dynamics in Halide Perovskites. Nano Letters, 2018, 18, 8041-8046.	4.5	97
74	Oxide chemistry and local structure of PbZrxTi1-xO3 studied by density-functional theory supercell calculations. Physical Review B, 2004, 69, .	1.1	92
75	Transferable relativistic Dirac-Slater pseudopotentials. Physical Review B, 2000, 62, 2311-2314.	1.1	91
76	A Pd-doped perovskite catalyst, BaCe1â^'xPdxO3â^'Î´BaCe1â^'xPdxO3â^'Î´, for CO oxidation. Journal of Catalysis, 2007, 249, 349-358.	3.1	91
77	Polarization Effects on the Surface Chemistry ofPbTiO3-Supported Pt Films. Physical Review Letters, 2007, 98, 166101.	2.9	86
78	Unusually Large Youngâ€™s Moduli of Amino Acid Molecular Crystals. Angewandte Chemie - International Edition, 2015, 54, 13566-13570.	7.2	83
79	Strain-Induced Ferroelectric Topological Insulator. Nano Letters, 2016, 16, 1663-1668.	4.5	82
80	Large-area synthesis of high-quality monolayer 1Tâ€™-WTe ₂ flakes. 2D Materials, 2017, 4, 021008.	2.0	81
81	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
82	Development of a bond-valence molecular-dynamics model for complex oxides. Physical Review B, 2005, 71, .	1.1	78
83	Band-gap engineering via local environment in complex oxides. Physical Review B, 2011, 83, .	1.1	77
84	Correlations between tetragonality, polarization, and ionic displacement in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>PbTiO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:m ferroelectric perovskite solid solutions. Physical Review B, 2010, 82, .	1.1	76
85	Two-Dimensionalï€-Conjugated Covalent-Organic Frameworks as Quantum Anomalous Hall Topological Insulators. Physical Review Letters, 2016, 116, 096601.	2.9	75
86	Anisotropic Local Correlations and Dynamics in a Relaxor Ferroelectric. Physical Review Letters, 2013, 110, 147602.	2.9	74
87	The Significance of Polarons and Dynamic Disorder in Halide Perovskites. ACS Energy Letters, 2021, 6, 2162-2173.	8.8	74
88	Photoferroelectric and Photopiezoelectric Properties of Organometal Halide Perovskites. Journal of Physical Chemistry Letters, 2016, 7, 1460-1465.	2.1	73
89	NonmonotonicTCTrends in Bi-Based Ferroelectric Perovskite Solid Solutions. Physical Review Letters, 2007, 98, 037603.	2.9	68
90	Effect of Particle Size on the Adsorption of O and S Atoms on Pt:Â A Density-Functional Theory Study. Journal of Physical Chemistry B, 2001, 105, 7739-7747.	1.2	65

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91	Correlated polarization switching in the proximity of a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>180</mml:mn><mml:mo>Â°</mml:mo></mml:mrow></mml:math>domain wall. Physical Review B, 2010, 82, .	1.1	65
92	Optimization of quantum Monte Carlo wave functions using analytical energy derivatives. Journal of Chemical Physics, 2000, 112, 2650-2654.	1.2	63
93	Molecular Dynamics Study of Dielectric Response in a Relaxor Ferroelectric. Physical Review Letters, 2009, 103, 197601.	2.9	62
94	Substantial bulk photovoltaic effect enhancement via nanolayering. Nature Communications, 2016, 7, 10419.	5.8	62
95	Enhancement of the Bulk Photovoltaic Effect in Topological Insulators. Physical Review Letters, 2016, 116, 237402.	2.9	61
96	Large polarization gradients and temperature-stable responses in compositionally-graded ferroelectrics. Nature Communications, 2017, 8, 14961.	5.8	60
97	Strongly Anharmonic Octahedral Tilting in Two-Dimensional Hybrid Halide Perovskites. ACS Nano, 2021, 15, 10153-10162.	7.3	59
98	Relationship between Local Structure and Relaxor Behavior in Perovskite Oxides. Physical Review Letters, 2007, 99, 267603.	2.9	58
99	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
100	The structural diversity of ABS3 compounds with d electronic configuration for the B-cation. Journal of Chemical Physics, 2014, 140, 224703.	1.2	55
101	In Situ Bottom-up Synthesis of Porphyrin-Based Covalent Organic Frameworks. Journal of the American Chemical Society, 2019, 141, 19560-19564.	6.6	55
102	Physical Adsorption: Theory of van der Waals Interactions between Particles and Clean Surfaces. Physical Review Letters, 2014, 112, 106101.	2.9	54
103	Surface Pyroelectricity in Cubic SrTiO₃. Advanced Materials, 2019, 31, e1904733.	11.1	54
104	Silver solid solution piezoelectrics. Applied Physics Letters, 2004, 85, 1760-1762.	1.5	53
105	First-principles investigation of the highly tetragonal ferroelectric material<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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109	First principles calculations, crystal chemistry and properties of ferroelectric perovskites. Phase Transitions, 2007, 80, 351-368.	0.6	51
110	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></m : A comprehensive study on substitutional doping. Physical Review B, 2018, 98, .	1.1	51
111	Correlations between the structure and dielectric properties ofPb(Sc2/3W1/3)O3â€“Pb(Ti/Zr)O3relaxors. Physical Review B, 2004, 69, .	1.1	50
112	Reinterpretation of the bond-valence model with bond-order formalism: An improved bond-valence-based interatomic potential for PbTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 88, .	1.1	50
113	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
114	Pb-free semiconductor ferroelectrics: A theoretical study of Pd-substituted<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Ba</mml:mtext><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:msub><mml:mrow> Physical Review B, 2010, 82, .	1.1	48
115	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>(001)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo		

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127	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
128	First-principles calculation of the bulk photovoltaic effect in the polar compounds LiAsS2, LiAsSe2, and NaAsSe2. Journal of Chemical Physics, 2014, 141, 204704.	1.2	44
129	First principles study of carbon monoxide adsorption on zirconia-supported copper. Surface Science, 2001, 495, 44-50.	0.8	43
130	Self-Initiation Mechanism in Spontaneous Thermal Polymerization of Ethyl and n-Butyl Acrylate: A Theoretical Study. Journal of Physical Chemistry A, 2010, 114, 7975-7983.	1.1	43
131	Crystalline Bilayer Graphene with Preferential Stacking from Niâ€“Cu Gradient Alloy. ACS Nano, 2018, 12, 2275-2282.	7.3	43
132	Synthesis and Physical Properties of Phase-Engineered Transition Metal Dichalcogenide Monolayer Heterostructures. ACS Nano, 2017, 11, 8619-8627.	7.3	42
133	Water in hybrid perovskites: Bulk MAPbI3 degradation via super-hydrous state. APL Materials, 2019, 7, .	2.2	42
134	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
135	Widespread Negative Longitudinal Piezoelectric Responses in Ferroelectric Crystals with Layered Structures. Physical Review Letters, 2021, 126, 217601.	2.9	42
136	Adsorbateâ^'Adsorbate Interactions and Chemisorption at Different Coverages Studied by Accurate ab initio Calculations:Â CO on Transition Metal Surfacesâ€. Journal of Physical Chemistry B, 2006, 110, 3816-3822.	1.2	41
137	Hybrid density functional calculations of the band gap of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ga</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:msu Physical Review B, 2009, 80, .	1.1	41
138	Substrate-Adsorbate Coupling in CO-Adsorbed Copper. Physical Review Letters, 1996, 77, 5241-5244.	2.9	39
139	Backbiting and Î²-scission reactions in free-radical polymerization of methyl acrylate. International Journal of Quantum Chemistry, 2014, 114, 345-360.	1.0	38
140	Computational Evidence for Self-Initiation in Spontaneous High-Temperature Polymerization of Methyl Methacrylate. Journal of Physical Chemistry A, 2011, 115, 1125-1132.	1.1	37
141	Strong Reciprocal Interaction between Polarization and Surface Stoichiometry in Oxide Ferroelectrics. Nano Letters, 2014, 14, 6711-6717.	4.5	37
142	Material Innovation in Advancing Organometal Halide Perovskite Functionality. Journal of Physical Chemistry Letters, 2015, 6, 4862-4872.	2.1	37
143	Mix and Match: Organic and Inorganic Ions in the Perovskite Lattice. Advanced Materials, 2019, 31, e1802697.	11.1	37
144	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

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145	Shift-current bulk photovoltaic effect influenced by quasiparticle and exciton. Physical Review B, 2020, 101, .	1.1	37
146	Large Bulk Piezophotovoltaic Effect of Monolayer 2H-MoS₂. Journal of Physical Chemistry Letters, 2021, 12, 1244-1249.	2.1	37
147	Origin and structure of polar domains in doped molecular crystals. Nature Communications, 2016, 7, 13351.	5.8	36
148	Structure and vibrations of the vicinal copper (211) surface. Physical Review B, 1998, 57, 10062-10068.	1.1	34
149	Quantitative criteria for transferable pseudopotentials in density functional theory. Physical Review B, 2001, 63, .	1.1	34
150	Modeling Spin-Forbidden Monomer Self-Initiation Reactions in Spontaneous Free-Radical Polymerization of Acrylates and Methacrylates. Journal of Physical Chemistry A, 2014, 118, 9310-9318.	1.1	34
151	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></mml:msub></mml:mrow></mml:math> with Raman scattering. Physical Review Materials, 2020, 4, .	3.1	34
152	Electronic quantum Monte Carlo calculations of atomic forces, vibrations, and anharmonicities. Journal of Chemical Physics, 2005, 122, 244103.	1.2	32
153	Computational Study of the Self-Initiation Mechanism in Thermal Polymerization of Methyl Acrylate. Journal of Physical Chemistry A, 2009, 113, 10787-10794.	1.1	32
154	Hybrid functional pseudopotentials. Physical Review B, 2018, 97, .	1.1	32
155	Bioferroelectric Properties of Glycine Crystals. Journal of Physical Chemistry Letters, 2019, 10, 1319-1324.	2.1	32
156	Phonon-Assisted Ballistic Current from First-Principles Calculations. Physical Review Letters, 2021, 126, 177403.	2.9	32
157	A test of the utility of plane-waves for the study of molecules from first principles. Journal of the American Chemical Society, 1992, 114, 6466-6469.	6.6	31
158	Density functional study ofPbTiO3nanocapacitors with Pt and Au electrodes. Physical Review B, 2010, 82, .	1.1	31
159	Atomic sublattice decomposition of piezoelectric response in tetragonal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Pb</mml:mi><mml:mi>Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ba</mml:mi><mml:mi>Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>, and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi ma. Physical Review B, 2014, 89, .	1.1	31
160	Short-circuit boundary conditions in ferroelectricPbTiO3thin films. Physical Review B, 2006, 74, .	1.1	30
161	Computational Study of Chain Transfer to Monomer Reactions in High-Temperature Polymerization of Alkyl Acrylates. Journal of Physical Chemistry A, 2013, 117, 2605-2618.	1.1	30
162	Density functional theory study of hypothetical <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>PbTiO</mml:mtext><mml:mn>3</mml:mn></mml:msub></mml:math> oxysulfides. Physical Review B, 2014, 89, .	1.1	30

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163	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:math> Physical Review Applied, 2015, 4, .	1.5	30
164	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
165	Adding to the Perovskite Universe: Inverse-Hybrid Perovskites. ACS Energy Letters, 2017, 2, 2681-2685.	8.8	30
166	Ab Initio Simulation Explains the Enhancement of Catalytic Oxygen Evolution on CaMnO₃. ACS Catalysis, 2018, 8, 2218-2224.	5.5	30
167	Phonon Influence on Bulk Photovoltaic Effect in the Ferroelectric Semiconductor GeTe. Physical Review Letters, 2018, 121, 017402.	2.9	30
168	Long-lived polarization memory in the electronic states of lead-halide perovskites from local structural dynamics. Nature Communications, 2018, 9, 3531.	5.8	29
169	Epitaxial Strain Control of Relaxor Ferroelectric Phase Evolution. Advanced Materials, 2019, 31, e1901060.	11.1	29
170	Layered Topological Crystalline Insulators. Physical Review Letters, 2015, 115, 086802.	2.9	28
171	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
172	Orbital-Specific Analysis of CO Chemisorption on Transition-Metal Surfaces. Journal of Physical Chemistry C, 2008, 112, 1963-1966.	1.5	27
173	Optimized norm-conserving Hartree-Fock pseudopotentials for plane-wave calculations. Physical Review B, 2008, 77, .	1.1	27
174	Materials Design of Visible-Light Ferroelectric Photovoltaics from First Principles. Ferroelectrics, 2015, 483, 1-12.	0.3	27
175	Supported metal electronic structure: Implications for molecular adsorption. Physical Review B, 2005, 72, .	1.1	26
176	Orderâ€“disorder character of PbTiO₃. Journal of Physics Condensed Matter, 2008, 20, 015224.	0.7	26
177	Polarization Dependence of Palladium Deposition on Ferroelectric Lithium Niobate (0001) Surfaces. Physical Review Letters, 2011, 107, 076102.	2.9	26
178	Electron-beam-induced ferroelectric domain behavior in the transmission electron microscope: Toward deterministic domain patterning. Physical Review B, 2016, 94, .	1.1	26
179	Ab initioinvestigation of carbon-related defects in silicon. Physical Review B, 1993, 47, 12554-12557.	1.1	25
180	First-principles study of band gap engineering via oxygen vacancy doping in perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>A</mml:mi><mml:mi>B</mml:mi><mml:msup><mml:mi>B</mml:mi><mml:mo>â€²</mml:mo> xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>solid solutions. Physical Review B, 2011, 84, .	1.1	25

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181	Theoretical Model of Oxidative Adsorption of Water on a Highly Reduced Reconstructed Oxide Surface. Journal of Physical Chemistry Letters, 2014, 5, 3408-3414.	2.1	25
182	Frequency-dependent dielectric function of semiconductors with application to physisorption. Physical Review B, 2017, 95, .	1.1	25
183	3-dimensional photonic band structure. Optical and Quantum Electronics, 1992, 24, S273-S283.	1.5	24
184	Structural and vibrational properties of carbon monoxide adlayers on the copper (001) surface. Journal of Chemical Physics, 1999, 110, 4619-4633.	1.2	24
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