

Andrew M Rappe

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293
papers

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140
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307
ext. papers

24,589
ext. citations

8.6
avg, IF

7.21
L-index

#	Paper	IF	Citations
293	Optimized pseudopotentials. <i>Physical Review B</i> , 1990 , 41, 1227-1230	3.3	1876
292	Dirac semimetal in three dimensions. <i>Physical Review Letters</i> , 2012 , 108, 140405	7.4	1072
291	Perovskite oxides for visible-light-absorbing ferroelectric and photovoltaic materials. <i>Nature</i> , 2013 , 503, 509-12	50.4	883
290	Donor and acceptor modes in photonic band structure. <i>Physical Review Letters</i> , 1991 , 67, 3380-3383	7.4	663
289	Dirac Line Nodes in Inversion-Symmetric Crystals. <i>Physical Review Letters</i> , 2015 , 115, 036806	7.4	534
288	Local Polar Fluctuations in Lead Halide Perovskite Crystals. <i>Physical Review Letters</i> , 2017 , 118, 136001	7.4	374
287	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
286	Thin-film ferroelectric materials and their applications. <i>Nature Reviews Materials</i> , 2017 , 2,	73.3	350
285	Accurate theoretical analysis of photonic band-gap materials. <i>Physical Review B</i> , 1993 , 48, 8434-8437	3.3	343
284	Ferroelectric phase transition in individual single-crystalline BaTiO ₃ nanowires. <i>Nano Letters</i> , 2006 , 6, 735-9	11.5	342
283	Hybrid Organic-Inorganic Perovskites (HOIPs): Opportunities and Challenges. <i>Advanced Materials</i> , 2015 , 27, 5102-12	24	325
282	Stabilization of monodomain polarization in ultrathin PbTiO ₃ films. <i>Physical Review Letters</i> , 2006 , 96, 127601	7.4	318
281	Measurement of photonic band structure in a two-dimensional periodic dielectric array. <i>Physical Review Letters</i> , 1992 , 68, 2023-2026	7.4	303
280	First principles calculation of the shift current photovoltaic effect in ferroelectrics. <i>Physical Review Letters</i> , 2012 , 109, 116601	7.4	297
279	Electromagnetic Bloch waves at the surface of a photonic crystal. <i>Physical Review B</i> , 1991 , 44, 10961-10964	3.4	286
278	Existence of a photonic band gap in two dimensions. <i>Applied Physics Letters</i> , 1992 , 61, 495-497	3.4	283
277	Nucleation and growth mechanism of ferroelectric domain-wall motion. <i>Nature</i> , 2007 , 449, 881-4	50.4	280

276	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
275	Comprehensive defect suppression in perovskite nanocrystals for high-efficiency light-emitting diodes. <i>Nature Photonics</i> , 2021 , 15, 148-155	33.9	257
274	Ferroelectricity in ultrathin perovskite films. <i>Physical Review B</i> , 2005 , 72,	3.3	225
273	Power conversion efficiency exceeding the Shockley-Queisser limit in a ferroelectric insulator. <i>Nature Photonics</i> , 2016 , 10, 611-616	33.9	224
272	Structure and energetics of alkanethiol adsorption on the Au(111) surface. <i>Journal of Chemical Physics</i> , 2002 , 117, 825-833	3.9	215
271	Reversible chemical switching of a ferroelectric film. <i>Physical Review Letters</i> , 2009 , 102, 047601	7.4	208
270	Relationship between local structure and phase transitions of a disordered solid solution. <i>Nature</i> , 2002 , 419, 909-11	50.4	208
269	High Chloride Doping Levels Stabilize the Perovskite Phase of Cesium Lead Iodide. <i>Nano Letters</i> , 2016 , 16, 3563-70	11.5	208
268	Double Dirac Semimetals in Three Dimensions. <i>Physical Review Letters</i> , 2016 , 116, 186402	7.4	199
267	Designed nonlocal pseudopotentials for enhanced transferability. <i>Physical Review B</i> , 1999 , 59, 12471-12478	3.8	188
266	Direct in situ determination of the polarization dependence of physisorption on ferroelectric surfaces. <i>Nature Materials</i> , 2008 , 7, 473-7	27	184
265	Hybrid Organic-Inorganic Perovskites on the Move. <i>Accounts of Chemical Research</i> , 2016 , 49, 573-81	24.3	176
264	Ferroelectric polarization reversal via successive ferroelastic transitions. <i>Nature Materials</i> , 2015 , 14, 79-86	8.7	175
263	What Remains Unexplained about the Properties of Halide Perovskites?. <i>Advanced Materials</i> , 2018 , 30, e1800691	24	174
262	Predicting morphotropic phase boundary locations and transition temperatures in Pb- and Bi-based perovskite solid solutions from crystal chemical data and first-principles calculations. <i>Journal of Applied Physics</i> , 2005 , 98, 094111	2.5	171
261	Are Mobilities in Hybrid Organic-Inorganic Halide Perovskites Actually "High"?. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 4754-7	6.4	167
260	Monolayer Single-Crystal 1T'-MoTe2 Grown by Chemical Vapor Deposition Exhibits Weak Antilocalization Effect. <i>Nano Letters</i> , 2016 , 16, 4297-304	11.5	167
259	First-principles calculation of the bulk photovoltaic effect in bismuth ferrite. <i>Physical Review Letters</i> , 2012 , 109, 236601	7.4	166

258	Predicting synthesizability. <i>Journal Physics D: Applied Physics</i> , 2019 , 52,	3	161
257	Continuous growth of hexagonal graphene and boron nitride in-plane heterostructures by atmospheric pressure chemical vapor deposition. <i>ACS Nano</i> , 2013 , 7, 10129-38	16.7	156
256	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
255	Photonic bound states in periodic dielectric materials. <i>Physical Review B</i> , 1991 , 44, 13772-13774	3.3	147
254	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
253	New highly polar semiconductor ferroelectrics through d8 cation-O vacancy substitution into PbTiO ₃ : a theoretical study. <i>Journal of the American Chemical Society</i> , 2008 , 130, 17409-12	16.4	145
252	Rashba Effect in a Single Colloidal CsPbBr Perovskite Nanocrystal Detected by Magneto-Optical Measurements. <i>Nano Letters</i> , 2017 , 17, 5020-5026	11.5	143
251	Shift current bulk photovoltaic effect in polar materials—Hybrid and oxide perovskites and beyond. <i>Npj Computational Materials</i> , 2016 , 2,	10.9	142
250	Growth mechanism of hexagonal-shape graphene flakes with zigzag edges. <i>ACS Nano</i> , 2011 , 5, 9154-60	16.7	140
249	Terahertz field-induced ferroelectricity in quantum paraelectric SrTiO. <i>Science</i> , 2019 , 364, 1079-1082	33.3	129
248	Slush-like polar structures in single-crystal relaxors. <i>Nature</i> , 2017 , 546, 391-395	50.4	128
247	Bulk Dirac points in distorted spinels. <i>Physical Review Letters</i> , 2014 , 112, 036403	7.4	123
246	Ultrafast photovoltaic response in ferroelectric nanolayers. <i>Physical Review Letters</i> , 2012 , 108, 087601	7.4	123
245	Virtual-crystal approximation that works: Locating a compositional phase boundary in Pb(Zr _{1-x} Ti _x)O ₃ . <i>Physical Review B</i> , 2000 , 62, R743-R746	3.3	120
244	Structure and polarization in the high T _c ferroelectric Bi(Zn,Ti)O ₃ -PbTiO ₃ solid solutions. <i>Physical Review Letters</i> , 2007 , 98, 107601	7.4	118
243	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
242	Post density functional theoretical studies of highly polar semiconductive Pb(Ti _{1-x} Ni _x)O _{3-x} solid solutions: Effects of cation arrangement on band gap. <i>Physical Review B</i> , 2011 , 83,	3.3	117
241	Band gap engineering strategy via polarization rotation in perovskite ferroelectrics. <i>Applied Physics Letters</i> , 2014 , 104, 152903	3.4	114

240	Theory of hydrogen migration in organic-inorganic halide perovskites. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 12437-41	16.4	112
239	Light-induced picosecond rotational disordering of the inorganic sublattice in hybrid perovskites. <i>Science Advances</i> , 2017 , 3, e1602388	14.3	109
238	Ferroelectrically driven spatial carrier density modulation in graphene. <i>Nature Communications</i> , 2015 , 6, 6136	17.4	107
237	Observation of surface photons on periodic dielectric arrays. <i>Optics Letters</i> , 1993 , 18, 528-30	3	107
236	Local structure and macroscopic properties in $\text{PbMg}_{1-x}\text{Nb}_2\text{B}_2\text{O}_{10}\text{PbTiO}_3$ and $\text{PbZn}_{1-x}\text{Nb}_2\text{B}_2\text{O}_{10}\text{PbTiO}_3$ solid solutions. <i>Physical Review B</i> , 2004 , 70,	3.3	104
235	Intrinsic ferroelectric switching from first principles. <i>Nature</i> , 2016 , 534, 360-3	50.4	101
234	Lattice normal modes and electronic properties of the correlated metal LaNiO_3 . <i>Physical Review B</i> , 2011 , 84,	3.3	98
233	Polarization Dependence of Water Adsorption to $\text{CH}_3\text{NH}_3\text{PbI}_3$ (001) Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 4371-8	6.4	93
232	CO on Pt(111) puzzle: A possible solution. <i>Journal of Chemical Physics</i> , 2002 , 117, 2264-2270	3.9	93
231	Theoretical investigation of the evolution of the topological phase of Bi_2Se_3 under mechanical strain. <i>Physical Review B</i> , 2011 , 84,	3.3	91
230	Influence of ferroelectric polarization on the equilibrium stoichiometry of lithium niobate (0001) surfaces. <i>Physical Review Letters</i> , 2008 , 100, 256101	7.4	91
229	Evolution of the structure and thermodynamic stability of the BaTiO_3 (001) surface. <i>Physical Review Letters</i> , 2008 , 101, 036102	7.4	91
228	Enhancing ferroelectric photovoltaic effect by polar order engineering. <i>Science Advances</i> , 2018 , 4, eaat3418	14.8	88
227	Collective coherent control: synchronization of polarization in ferroelectric PbTiO_3 by shaped THz fields. <i>Physical Review Letters</i> , 2009 , 102, 247603	7.4	88
226	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
225	Transferable relativistic Dirac-Slater pseudopotentials. <i>Physical Review B</i> , 2000 , 62, 2311-2314	3.3	82
224	Oxide chemistry and local structure of $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$ studied by density-functional theory supercell calculations. <i>Physical Review B</i> , 2004 , 69,	3.3	79
223	A Pd-doped perovskite catalyst, $\text{BaCe}_{1-x}\text{Pd}_x\text{O}_3$ for CO oxidation. <i>Journal of Catalysis</i> , 2007 , 249, 349-358	7.3	77

222	Wallpaper fermions and the nonsymmorphic Dirac insulator. <i>Science</i> , 2018 , 361, 246-251	33.3	73
221	Polarization effects on the surface chemistry of PbTiO ₃ -supported Pt films. <i>Physical Review Letters</i> , 2007 , 98, 166101	7.4	72
220	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
219	Strain-Induced Ferroelectric Topological Insulator. <i>Nano Letters</i> , 2016 , 16, 1663-8	11.5	67
218	Topological Semimetals from First Principles. <i>Annual Review of Materials Research</i> , 2019 , 49, 153-183	12.8	67
217	Band-gap engineering via local environment in complex oxides. <i>Physical Review B</i> , 2011 , 83,	3.3	67
216	Two-Dimensional π -Conjugated Covalent-Organic Frameworks as Quantum Anomalous Hall Topological Insulators. <i>Physical Review Letters</i> , 2016 , 116, 096601	7.4	65
215	Development of a bond-valence molecular-dynamics model for complex oxides. <i>Physical Review B</i> , 2005 , 71,	3.3	65
214	Anisotropic local correlations and dynamics in a relaxor ferroelectric. <i>Physical Review Letters</i> , 2013 , 110, 147602	7.4	64
213	Correlations between tetragonality, polarization, and ionic displacement in PbTiO ₃ -derived ferroelectric perovskite solid solutions. <i>Physical Review B</i> , 2010 , 82,	3.3	64
212	Effect of Particle Size on the Adsorption of O and S Atoms on Pt: A Density-Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 7739-7747	3.4	62
211	Optimization of quantum Monte Carlo wave functions using analytical energy derivatives. <i>Journal of Chemical Physics</i> , 2000 , 112, 2650-2654	3.9	60
210	Photoferroelectric and Photopiezoelectric Properties of Organometal Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 1460-5	6.4	59
209	Spatially dispersive circular photogalvanic effect in a Weyl semimetal. <i>Nature Materials</i> , 2019 , 18, 955-962	7	58
208	Correlated polarization switching in the proximity of a 180° domain wall. <i>Physical Review B</i> , 2010 , 82,	3.3	58
207	Large-area synthesis of high-quality monolayer 1T'-WTe flakes. <i>2D Materials</i> , 2017 , 4,	5.9	56
206	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
205	Mixed Valence Perovskite Cs ₂ AuI ₃ : A Potential Material for Thin-Film Pb-Free Photovoltaic Cells with Ultrahigh Efficiency. <i>Advanced Materials</i> , 2018 , 30, e1707001	24	54

204	Unusually Large Young's Moduli of Amino Acid Molecular Crystals. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 13566-70	16.4	54
203	Nonmonotonic TC trends in bi-based ferroelectric perovskite solid solutions. <i>Physical Review Letters</i> , 2007 , 98, 037603	7.4	54
202	Molecular dynamics study of dielectric response in a relaxor ferroelectric. <i>Physical Review Letters</i> , 2009 , 103, 197601	7.4	52
201	Relationship between local structure and relaxor behavior in perovskite oxides. <i>Physical Review Letters</i> , 2007 , 99, 267603	7.4	52
200	Substantial bulk photovoltaic effect enhancement via nanolayering. <i>Nature Communications</i> , 2016 , 7, 10419	17.4	51
199	How Lattice and Charge Fluctuations Control Carrier Dynamics in Halide Perovskites. <i>Nano Letters</i> , 2018 , 18, 8041-8046	11.5	51
198	First-principles investigation of the highly tetragonal ferroelectric material $\text{Bi}(\text{Zn}_{1/2}\text{Ti}_{1/2})\text{O}_3$. <i>Physical Review B</i> , 2009 , 79,	3.3	50
197	Silver solid solution piezoelectrics. <i>Applied Physics Letters</i> , 2004 , 85, 1760-1762	3.4	48
196	First-principles calculation of the bulk photovoltaic effect in KNbO_3 and $(\text{K,Ba})(\text{Ni,Nb})\text{O}_3$. <i>Physical Review B</i> , 2015 , 91,	3.3	47
195	Atomic and Electronic Structure of the $\text{BaTiO}_3(001)$ ($\sqrt{5} \times \sqrt{5}$) $\times R26.6^\circ$ Surface Reconstruction. <i>Physical Review Letters</i> , 2012 , 109, 256802	7.4	47
194	Pb-free semiconductor ferroelectrics: A theoretical study of Pd-substituted $\text{Ba}(\text{Ti}_{1-x}\text{Cex})\text{O}_3$ solid solutions. <i>Physical Review B</i> , 2010 , 82,	3.3	45
193	Physical adsorption: theory of van der Waals interactions between particles and clean surfaces. <i>Physical Review Letters</i> , 2014 , 112, 106101	7.4	44
192	Correlations between the structure and dielectric properties of $\text{Pb}(\text{Sc}_{2/3}\text{W}_{1/3})\text{O}_3$ / $\text{Pb}(\text{Ti/Zr})\text{O}_3$ relaxors. <i>Physical Review B</i> , 2004 , 69,	3.3	44
191	Computing accurate forces in quantum Monte Carlo using Pulay's corrections and energy minimization. <i>Journal of Chemical Physics</i> , 2003 , 118, 7193	3.9	44
190	Large polarization gradients and temperature-stable responses in compositionally-graded ferroelectrics. <i>Nature Communications</i> , 2017 , 8, 14961	17.4	43
189	$\text{BaCe}_{1-x}\text{Pd}_x\text{O}_3$ ($0 \leq x \leq 0.1$): Redox Controlled Ingress and Egress of Palladium in a Perovskite. <i>Chemistry of Materials</i> , 2007 , 19, 1418-1426	9.6	43
188	Spin texture on the Fermi surface of tensile-strained HgTe. <i>Physical Review B</i> , 2013 , 87,	3.3	42
187	Reinterpretation of the bond-valence model with bond-order formalism: An improved bond-valence-based interatomic potential for PbTiO_3 . <i>Physical Review B</i> , 2013 , 88,	3.3	40

186	Rigorous definition of oxidation states of ions in solids. <i>Physical Review Letters</i> , 2012 , 108, 166403	7.4	39
185	Hybrid density functional calculations of the band gap of GaIn _{1-x} N. <i>Physical Review B</i> , 2009 , 80,	3.3	39
184	Substrate-Adsorbate Coupling in CO-Adsorbed Copper. <i>Physical Review Letters</i> , 1996 , 77, 5241-5244	7.4	39
183	Semiconducting ferroelectric photovoltaics through Zn ²⁺ doping into KNbO ₃ and polarization rotation. <i>Physical Review B</i> , 2014 , 89,	3.3	38
182	The structural diversity of ABX ₃ compounds with d ⁰ electronic configuration for the B-cation. <i>Journal of Chemical Physics</i> , 2014 , 140, 224703	3.9	38
181	Self-initiation mechanism in spontaneous thermal polymerization of ethyl and n-butyl acrylate: a theoretical study. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 7975-83	2.8	38
180	First principles calculations, crystal chemistry and properties of ferroelectric perovskites. <i>Phase Transitions</i> , 2007 , 80, 351-368	1.3	37
179	First principles study of carbon monoxide adsorption on zirconia-supported copper. <i>Surface Science</i> , 2001 , 495, 44-50	1.8	37
178	Adsorbate-adsorbate interactions and chemisorption at different coverages studied by accurate ab initio calculations: CO on transition metal surfaces. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 3816-22	3.4	36
177	Doping of BiFeO ₃ : A comprehensive study on substitutional doping. <i>Physical Review B</i> , 2018 , 98,	3.3	36
176	Material Innovation in Advancing Organometal Halide Perovskite Functionality. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 4862-72	6.4	35
175	Enhancement of the Bulk Photovoltaic Effect in Topological Insulators. <i>Physical Review Letters</i> , 2016 , 116, 237402	7.4	34
174	Synthesis and Physical Properties of Phase-Engineered Transition Metal Dichalcogenide Monolayer Heterostructures. <i>ACS Nano</i> , 2017 , 11, 8619-8627	16.7	34
173	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
172	Development of a bond-valence based interatomic potential for BiFeO ₃ for accurate molecular dynamics simulations. <i>Journal of Physics Condensed Matter</i> , 2013 , 25, 102202	1.8	34
171	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
170	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
169	Stable Phosphorus-Enriched (0001) Surfaces of Nickel Phosphides. <i>Chemistry of Materials</i> , 2016 , 28, 5365-5372	3.3	33

168	Computational evidence for self-initiation in spontaneous high-temperature polymerization of methyl methacrylate. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 1125-32	2.8	33
167	Quantitative criteria for transferable pseudopotentials in density functional theory. <i>Physical Review B</i> , 2001 , 63,	3.3	33
166	Structure and vibrations of the vicinal copper (211) surface. <i>Physical Review B</i> , 1998 , 57, 10062-10068	3.3	33
165	Crystalline Bilayer Graphene with Preferential Stacking from Ni-Cu Gradient Alloy. <i>ACS Nano</i> , 2018 , 12, 2275-2282	16.7	32
164	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
163	First-principles calculation of the bulk photovoltaic effect in the polar compounds LiAsS ₂ , LiAsSe ₂ , and NaAsSe ₂ . <i>Journal of Chemical Physics</i> , 2014 , 141, 204704	3.9	31
162	Computational study of the self-initiation mechanism in thermal polymerization of methyl acrylate. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 10787-94	2.8	30
161	Electronic quantum Monte Carlo calculations of atomic forces, vibrations, and anharmonicities. <i>Journal of Chemical Physics</i> , 2005 , 122, 244103	3.9	30
160	Surface Pyroelectricity in Cubic SrTiO ₃ . <i>Advanced Materials</i> , 2019 , 31, e1904733	24	29
159	Strong reciprocal interaction between polarization and surface stoichiometry in oxide ferroelectrics. <i>Nano Letters</i> , 2014 , 14, 6711-7	11.5	29
158	A test of the utility of plane-waves for the study of molecules from first principles. <i>Journal of the American Chemical Society</i> , 1992 , 114, 6466-6469	16.4	29
157	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
156	Kinetic control of tunable multi-state switching in ferroelectric thin films. <i>Nature Communications</i> , 2019 , 10, 1282	17.4	28
155	Atomistic description for temperature-driven phase transitions in BaTiO ₃ . <i>Physical Review B</i> , 2016 , 94,	3.3	28
154	Density functional study of PbTiO ₃ nanocapacitors with Pt and Au electrodes. <i>Physical Review B</i> , 2010 , 82,	3.3	28
153	Short-circuit boundary conditions in ferroelectric PbTiO ₃ thin films. <i>Physical Review B</i> , 2006 , 74,	3.3	28
152	Materials Design of Visible-Light Ferroelectric Photovoltaics from First Principles. <i>Ferroelectrics</i> , 2015 , 483, 1-12	0.6	27
151	Computational study of chain transfer to monomer reactions in high-temperature polymerization of alkyl acrylates. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 2605-18	2.8	27

150	Modeling spin-forbidden monomer self-initiation reactions in spontaneous free-radical polymerization of acrylates and methacrylates. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 9310-8	2.8	26
149	First-Principles Materials Design of High-Performing Bulk Photovoltaics with the LiNbO ₃ Structure. <i>Physical Review Applied</i> , 2015 , 4,	4.3	26
148	Atomic sublattice decomposition of piezoelectric response in tetragonal PbTiO ₃ , BaTiO ₃ , and KNbO ₃ . <i>Physical Review B</i> , 2014 , 89,	3.3	26
147	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
146	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
145	Water in hybrid perovskites: Bulk MAPbI ₃ degradation via super-hydrous state. <i>APL Materials</i> , 2019 , 7, 041112	5.7	25
144	Large-area epitaxial growth of curvature-stabilized ABC trilayer graphene. <i>Nature Communications</i> , 2020 , 11, 546	17.4	25
143	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
142	Polarization dependence of palladium deposition on ferroelectric lithium niobate (0001) surfaces. <i>Physical Review Letters</i> , 2011 , 107, 076102	7.4	25
141	Supported metal electronic structure: Implications for molecular adsorption. <i>Physical Review B</i> , 2005 , 72,	3.3	25
140	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
139	Layered Topological Crystalline Insulators. <i>Physical Review Letters</i> , 2015 , 115, 086802	7.4	24
138	First-principles study of band gap engineering via oxygen vacancy doping in perovskite ABB ₂ O ₃ solid solutions. <i>Physical Review B</i> , 2011 , 84,	3.3	24
137	Origin and structure of polar domains in doped molecular crystals. <i>Nature Communications</i> , 2016 , 7, 13351	17.4	24
136	Orbital-Specific Analysis of CO Chemisorption on Transition-Metal Surfaces. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 1963-1966	3.8	23
135	Ab initio investigation of carbon-related defects in silicon. <i>Physical Review B</i> , 1993 , 47, 12554-12557	3.3	23
134	Mix and Match: Organic and Inorganic Ions in the Perovskite Lattice. <i>Advanced Materials</i> , 2019 , 31, e1802697	26.7	23
133	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

132	Computational study of cyclohexanone-monomer co-initiation mechanism in thermal homo-polymerization of methyl acrylate and methyl methacrylate. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 5337-48	2.8	22
131	Structural and vibrational properties of carbon monoxide adlayers on the copper (001) surface. <i>Journal of Chemical Physics</i> , 1999 , 110, 4619-4633	3.9	22
130	Shift-current bulk photovoltaic effect influenced by quasiparticle and exciton. <i>Physical Review B</i> , 2020 , 101,	3.3	21
129	Optimized norm-conserving Hartree-Fock pseudopotentials for plane-wave calculations. <i>Physical Review B</i> , 2008 , 77,	3.3	21
128	3-dimensional photonic band structure. <i>Optical and Quantum Electronics</i> , 1992 , 24, S273-S283	2.4	21
127	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
126	Adding to the Perovskite Universe: Inverse-Hybrid Perovskites. <i>ACS Energy Letters</i> , 2017 , 2, 2681-2685	20.1	20
125	Epitaxial Strain Control of Relaxor Ferroelectric Phase Evolution. <i>Advanced Materials</i> , 2019 , 31, e1901060	4	20
124	Structural and ferroelectric phase evolution in $[\text{KNbO}_3]_{1-x}[\text{BaNi}_{1/2}\text{Nb}_{1/2}\text{O}_3]_x$ ($x=0,0.1$). <i>Physical Review B</i> , 2017 , 96,	3.3	20
123	Order-disorder character of PbTiO_3 . <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 015224	1.8	20
122	Coadsorption of methyl radicals and oxygen on $\text{Rh}(111)$. <i>Surface Science</i> , 2004 , 549, 265-272	1.8	20
121	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
120	Semiconducting ferroelectric perovskites with intermediate bands via B-site Bi^{5+} doping. <i>Physical Review B</i> , 2014 , 90,	3.3	19
119	Coexisting surface phases and coherent one-dimensional interfaces on $\text{BaTiO}_3(001)$. <i>ACS Nano</i> , 2014 , 8, 4465-73	16.7	19
118	Pb-free ferroelectrics investigated with density functional theory: $\text{SnAl}_{1/2}\text{Nb}_{1/2}\text{O}_3$ perovskites. <i>Physical Review B</i> , 2011 , 83,	3.3	19
117	Continuum elastic theory of adsorbate vibrational relaxation. <i>Journal of Chemical Physics</i> , 1998 , 108, 1157-1161	3.9	19
116	Frequency-dependent dielectric function of semiconductors with application to physisorption. <i>Physical Review B</i> , 2017 , 95,	3.3	18
115	Density functional theory study of hypothetical PbTiO_3 -based oxysulfides. <i>Physical Review B</i> , 2014 , 89,	3.3	18

114	Screened van der Waals correction to density functional theory for solids. <i>Physical Review Materials</i> , 2017 , 1,	3.2	18
113	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
112	Bioferroelectric Properties of Glycine Crystals. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 1319-1324.	4.4	17
111	Ab Initio Simulation Explains the Enhancement of Catalytic Oxygen Evolution on CaMnO ₃ . <i>ACS Catalysis</i> , 2018 , 8, 2218-2224	13.1	17
110	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
109	On the Thermal Self-Initiation Reaction of n-Butyl Acrylate in Free-Radical Polymerization. <i>Processes</i> , 2018 , 6, 3	2.9	17
108	The Significance of Polarons and Dynamic Disorder in Halide Perovskites. <i>ACS Energy Letters</i> , 2021 , 6, 2162-2173	20.1	17
107	Phonon Influence on Bulk Photovoltaic Effect in the Ferroelectric Semiconductor GeTe. <i>Physical Review Letters</i> , 2018 , 121, 017402	7.4	17
106	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
105	First principles study of three-component SrTiO ₃ /BaTiO ₃ /PbTiO ₃ ferroelectric superlattices. <i>Journal of Materials Science</i> , 2008 , 43, 3750-3760	4.3	16
104	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
103	Ab initio study of silver niobate. <i>AIP Conference Proceedings</i> , 2003 ,	0	15
102	Strongly Anharmonic Octahedral Tilting in Two-Dimensional Hybrid Halide Perovskites. <i>ACS Nano</i> , 2021 , 15, 10153-10162	16.7	15
101	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
100	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
99	Ultrafast Electric Field Pulse Control of Giant Temperature Change in Ferroelectrics. <i>Physical Review Letters</i> , 2018 , 120, 055901	7.4	14
98	First-principles studies of the local structure and relaxor behavior of Pb(Mg _{1/3} Nb _{2/3})O ₃ /PbTiO ₃ -derived ferroelectric perovskite solid solutions. <i>Physical Review B</i> , 2018 , 97,	3.3	14
97	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

96	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
95	Theoretical examination of stress fields in Pb(Zr _{0.5} Ti _{0.5})O ₃ . <i>Ferroelectrics</i> , 1998 , 206, 31-46	0.6	14
94	Asymmetry in mechanical polarization switching. <i>Applied Physics Letters</i> , 2017 , 110, 222903	3.4	13
93	Hybrid functional pseudopotentials. <i>Physical Review B</i> , 2018 , 97,	3.3	13
92	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
91	Exploration of the intrinsic inertial response of ferroelectric domain walls via molecular dynamics simulations. <i>Applied Physics Letters</i> , 2013 , 103, 232907	3.4	13
90	Collective Motion and Structural Order in Adsorbate Vibrational Dynamics. <i>Physical Review Letters</i> , 1998 , 81, 5940-5943	7.4	13
89	Ab initio study of a grain boundary in gold. <i>Physical Review B</i> , 1992 , 46, 9768-9771	3.3	13
88	Study of n-Butyl Acrylate Self-Initiation Reaction Experimentally and via Macroscopic Mechanistic Modeling. <i>Processes</i> , 2016 , 4, 15	2.9	13
87	Theoretical study of chain transfer to solvent reactions of alkyl acrylates. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 5474-87	2.8	12
86	Controlling oxide surface dipole and reactivity with intrinsic nonstoichiometric epitaxial reconstructions. <i>Physical Review B</i> , 2015 , 92,	3.3	12
85	Giant Bulk Photovoltaic Effect in Vinylene-Linked Hybrid Heterocyclic Polymer. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 6500-6507	3.8	11
84	Upper limit on shift current generation in extended systems. <i>Physical Review B</i> , 2019 , 100,	3.3	11
83	Stabilization of highly polarized PbTiO ₃ nanoscale capacitors due to in-plane symmetry breaking at the interface. <i>Physical Review B</i> , 2012 , 85,	3.3	11
82	Ab initio optimized pseudopotential calculations of magnetic systems. <i>Physical Review B</i> , 1995 , 52, 12760-12765	3.1	11
81	Large Bulk Piezophotovoltaic Effect of Monolayer 2-MoS. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 1244-1249	6.4	11
80	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
79	Tuning the gap of lead-based halide perovskites by introducing superalkali species at the cationic sites of ABX-type structure. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 20619-20626	3.6	10

78	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
77	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
76	Anion Exchange in II-VI Semiconducting Nanostructures via Atomic Templating. <i>Nano Letters</i> , 2018 , 18, 1620-1627	11.5	9
75	Surface Chemically Switchable Ultraviolet Luminescence from Interfacial Two-Dimensional Electron Gas. <i>Nano Letters</i> , 2016 , 16, 681-7	11.5	9
74	Enhanced charge ordering transition in doped CaFeO ₃ through steric templating. <i>Physical Review B</i> , 2014 , 89,	3.3	9
73	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
72	Unusually Large Young's Moduli of Amino Acid Molecular Crystals. <i>Angewandte Chemie</i> , 2015 , 127, 13770-13774	13.7	9
71	Nonmonotonic Composition Dependence of the Dielectric Response of Ba _{1-x} CaxZrO ₃ . <i>Chemistry of Materials</i> , 2008 , 20, 5134-5138	9.6	9
70	Transition metal inverse-hybrid perovskites. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 14560-14565	13	9
69	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
68	Asymmetric Response of Ferroelastic Domain-Wall Motion under Applied Bias. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 2935-41	9.5	8
67	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
66	Electronic transition above room temperature in CaMn ₇ O ₁₂ films. <i>Applied Physics Letters</i> , 2015 , 107, 142901	3.4	8
65	Multiple dielectric transitions in the PbTiO ₃ -Bi(Zn _{1/2} Ti _{1/2})O ₃ -Bi(Mg _{1/2} Ti _{1/2})O ₃ system. <i>Journal of Applied Physics</i> , 2011 , 110, 074110	2.5	8
64	Spontaneous formation of dipolar metal nanoclusters. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 4134-4138	7.8	8
63	Investigation of chemisorbed molecular states for oxygen on rhodium (111). <i>Journal of Chemical Physics</i> , 2000 , 113, 4388-4391	3.9	8
62	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
61	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

60	Shift photovoltaic current and magnetically induced bulk photocurrent in piezoelectric sillenite crystals. <i>Physical Review B</i> , 2020 , 102,	3.3	8
59	Phonon-Assisted Ballistic Current from First-Principles Calculations. <i>Physical Review Letters</i> , 2021 , 126, 177403	7.4	8
58	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
57	Origin of the anomalous Pb-Br bond dynamics in formamidinium lead bromide perovskites. <i>Physical Review B</i> , 2020 , 101,	3.3	7
56	Design of Metal-Halide Inverse-Hybrid Perovskites. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 13872-13883	9.8	7
55	Method of Moments Applied to Most-Likely High-Temperature Free-Radical Polymerization Reactions. <i>Processes</i> , 2019 , 7, 656	2.9	7
54	Computational Studies of Lead-based Relaxor Ferroelectrics. <i>Ferroelectrics</i> , 2014 , 469, 1-13	0.6	7
53	Theory of Hydrogen Migration in Organic-Inorganic Halide Perovskites. <i>Angewandte Chemie</i> , 2015 , 127, 12614-12618	3.6	7
52	Coupling between octahedral rotations and local polar displacements in WO ₃ /ReO ₃ superlattices. <i>Physical Review B</i> , 2014 , 89,	3.3	7
51	Stress-induced phase transition in Pb(Zr _{1/2} Ti _{1/2})O ₃ 1998 ,		7
50	Widespread Negative Longitudinal Piezoelectric Responses in Ferroelectric Crystals with Layered Structures. <i>Physical Review Letters</i> , 2021 , 126, 217601	7.4	7
49	Assemblage of Superalkali Complexes with Ever Low-Ionization Potentials. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 6493-9	2.8	7
48	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
47	Molecule-Adsorbed Topological Insulator and Metal Surfaces: A Comparative First-Principles Study. <i>Chemistry of Materials</i> , 2018 , 30, 1849-1855	9.6	6
46	Valence Band Control of Metal Silicide Films via Stoichiometry. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 2573-8	6.4	6
45	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
44	Metal cation s lone-pairs increase octahedral tilting instabilities in halide perovskites. <i>Materials Advances</i> , 2021 , 2, 4610-4616	3.3	6
43	Novel materials solutions and simulations for nanoelectromechanical switches 2015 ,		5

42	Variational Monte Carlo calculation of the spin gap in the $\nu=1$ quantum Hall liquid. <i>Physical Review B</i> , 1997 , 56, 4760-4771	3.3	5
41	Force calculation of polyatomic molecules in quantum Monte Carlo using Pulay's corrections. <i>Molecular Physics</i> , 2007 , 105, 2493-2497	1.7	5
40	Effect of wavefunction delocalization on shift current generation. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 084002	1.8	5
39	Seeing the forest and the trees. <i>Nature Materials</i> , 2018 , 17, 657-658	27	5
38	Adsorption of Benzene on the RuO ₂ (110) Surface. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 1585-1590	3.8	4
37	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
36	PREDICTION OF DIELECTRIC DISPERSION FOR LEAD BASED PEROVSKITES AND STUDY OF LOCAL DIELECTRIC RESPONSE IN 0.75Pb(Mg ^{1/3} Nb ^{2/3})O ₃ 0.25PbTiO ₃ . <i>Journal of Advanced Dielectrics</i> , 2012 , 02, 1241009	1.3	4
35	Extending first principles modeling with crystal chemistry: a bond-valence based classical potential. <i>AIP Conference Proceedings</i> , 2003 ,	0	4
34	Efficient scaling of calculations involving separable nonlocal potentials. <i>Physical Review B</i> , 1998 , 58, 3482-3485	3.3	4
33	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
32	Ferroelectric barium titanate derivatives containing Mo and Mg for transparent photovoltaic applications. <i>Journal of Applied Physics</i> , 2019 , 126, 174101	2.5	4
31	Big data approach for effective ionic radii. <i>Computer Physics Communications</i> , 2019 , 237, 238-243	4.2	4
30	Ideal near-Dirac triple-point semimetal in III-V semiconductor alloys. <i>Physical Review B</i> , 2020 , 101,	3.3	3
29	Modified Schottky emission to explain thickness dependence and slow depolarization in BaTiO ₃ nanowires. <i>Physical Review B</i> , 2015 , 91,	3.3	3
28	Intrinsic Fermi-surface contribution to the bulk photovoltaic effect. <i>Physical Review Research</i> , 2021 , 3,	3.9	3
27	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
26	Mechanochemical Effects of Adsorbates at Nanoelectromechanical Switch Contacts. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 39238-39247	9.5	2
25	Theoretical examination of picosecond phenol migration dynamics in phenylacetylene solution. <i>Chemical Physics</i> , 2013 , 422, 175-183	2.3	2

24	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
23	Studies of Perovskite Materials for High-Performance Storage Media, Piezoelectric, and Solar Energy Conversion Devices 2010 ,		2
22	Macroscopic mechanistic modeling and optimization of a self-initiated high-temperature polymerization reactor 2011 ,		2
21	New Prospects for High Performance SONAR, Chemical Sensor, and Communication Device Materials 2009 ,		2
20	Adsorbate aggregation and relaxation of low-frequency vibrations. <i>Journal of Chemical Physics</i> , 2000 , 113, 10265-10271	3.9	2
19	Mixed-basis pseudopotential method applied to iterative diagonalization techniques. <i>Physical Review B</i> , 1992 , 46, 7353-7357	3.3	2
18	Bond-Valence Model of Ferroelectric PbTiO ₃ . <i>Journal of the Korean Physical Society</i> , 2008 , 52, 1206-1210.	0.6	2
17	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
16	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
15	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
14	Reply to 'Reconsidering the Shockley-Queisser limit of a ferroelectric insulator device'. <i>Nature Photonics</i> , 2017 , 11, 330-330	33.9	1
13	Substantial optical dielectric enhancement by volume compression in LiAsSe ₂ . <i>Physical Review B</i> , 2016 , 93,	3.3	1
12	Kinetics of palladium particles on LiNbO ₃ : an origin of the polarization-dependent catalysis. <i>Materials Research Society Symposia Proceedings</i> , 2012 , 1397, 1		1
11	Reciprocity theorems and pseudoelectric fields for ab initio force calculations. <i>Physical Review B</i> , 1997 , 55, 15356-15359	3.3	1
10	Bonding and Vibrational Properties of CO-adsorbed Copper. <i>Materials Research Society Symposia Proceedings</i> , 1995 , 408, 391		1
9	Ferroelectric Switching of Pure Spin Polarization in Two-Dimensional Electron Gas. <i>Nano Letters</i> , 2020 , 20, 7230-7236	11.5	1
8	Spin-orbit enhanced carrier lifetimes in noncentrosymmetric semiconductors. <i>Journal of Physics and Chemistry of Solids</i> , 2019 , 128, 225-230	3.9	1
7	Stromataxic Stabilization of a Metastable Layered ScFeO ₃ Polymorph. <i>Chemistry of Materials</i> , 2021 , 33, 7423-7431	9.6	1

6	Theoretical Insights Into Thermal Self-Initiation Reactions of Acrylates 2019 , 99-134	0
5	Oxygen-Initiated Free-Radical Polymerization of Alkyl Acrylates at High Temperatures. <i>Macromolecules</i> , 2021 , 54, 7925-7930	5.5 0
4	Theoretical Insights Into Chain Transfer Reactions of Acrylates 2019 , 135-193	
3	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
2	Electronic Quantum Monte Carlo Calculations of Energies and Atomic Forces for Diatomic and Polyatomic Molecules. <i>ACS Symposium Series</i> , 2006 , 69-79	0.4
1	Hydrogen freedom linked to perovskite efficiency. <i>Nature Materials</i> , 2021 , 20, 914-915	27