David Vanderbilt

List of Publications by Year
in descending order

297 papers	77,117 citations	1792 103 h-index	449 273 g-index
301 all docs	301 docs citations	301 times ranked	38454 citing authors

#	Article	IF	Citations
1	Soft self-consistent pseudopotentials in a generalized eigenvalue formalism. Physical Review B, 1990, 41, 7892-7895.	1.1	20,195
2	Maximally localized generalized Wannier functions for composite energy bands. Physical Review B, 1997, 56, 12847-12865.	1.1	3,642
3	Theory of polarization of crystalline solids. Physical Review B, 1993, 47, 1651-1654.	1.1	3,373
4	wannier90: A tool for obtaining maximally-localised Wannier functions. Computer Physics Communications, 2008, 178, 685-699.	3.0	2,947
5	Spontaneous polarization and piezoelectric constants of III-V nitrides. Physical Review B, 1997, 56, R10024-R10027.	1.1	2,662
6	Maximally localized Wannier functions: Theory and applications. Reviews of Modern Physics, 2012, 84, 1419-1475.	16.4	2,159
7	An updated version of wannier90: A tool for obtaining maximally-localised Wannier functions. Computer Physics Communications, 2014, 185, 2309-2310.	3.0	1,561
8	Maximally localized Wannier functions for entangled energy bands. Physical Review B, 2001, 65, .	1.1	1,546
9	Car-Parrinello molecular dynamics with Vanderbilt ultrasoft pseudopotentials. Physical Review B, 1993, 47, 10142-10153.	1.1	1,303
10	Pseudopotentials for high-throughput DFT calculations. Computational Materials Science, 2014, 81, 446-452.	1.4	1,114
11	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
12	Electric polarization as a bulk quantity and its relation to surface charge. Physical Review B, 1993, 48, 4442-4455.	1.1	1,016
13	Thermal Contraction and Disordering of the Al(110) Surface. Physical Review Letters, 1999, 82, 3296-3299.	2.9	929
14	Giant LO-TO splittings in perovskite ferroelectrics. Physical Review Letters, 1994, 72, 3618-3621.	2.9	834
15	Wannier90 as a community code: new features and applications. Journal of Physics Condensed Matter, 2020, 32, 165902.	0.7	807
16	Magnetoelectric Polarizability and Axion Electrodynamics in Crystalline Insulators. Physical Review Letters, 2009, 102, 146805.	2.9	766
17	Optimally smooth norm-conserving pseudopotentials. Physical Review B, 1985, 32, 8412-8415.	1.1	700
18	Systematic treatment of displacements, strains, and electric fields in density-functional perturbation theory. Physical Review B, 2005, 72, .	1.1	675

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19	Spontaneous Formation of Stress Domains on Crystal Surfaces. Physical Review Letters, 1988, 61, 1973-1976.	2.9	666
20	First-principles theory of ferroelectric phase transitions for perovskites: The case ofBaTiO3. Physical Review B, 1995, 52, 6301-6312.	1.1	649
21	Density-matrix electronic-structure method with linear system-size scaling. Physical Review B, 1993, 47, 10891-10894.	1.1	647
22	Virtual crystal approximation revisited: Application to dielectric and piezoelectric properties of perovskites. Physical Review B, 2000, 61, 7877-7882.	1.1	632
23	First-principles investigation of ferroelectricity in perovskite compounds. Physical Review B, 1994, 49, 5828-5844.	1.1	629
24	First-principles study of structural, vibrational, and lattice dielectric properties of hafnium oxide. Physical Review B, 2002, 65, .	1.1	623
25	Phase Transitions in BaTiO3from First Principles. Physical Review Letters, 1994, 73, 1861-1864.	2.9	589
26	Finite-Temperature Properties ofPb(Zr1â^'xTix)O3Alloys from First Principles. Physical Review Letters, 2000, 84, 5427-5430.	2.9	568
27	First-principles calculations of the energetics of stoichiometricTiO2surfaces. Physical Review B, 1994, 49, 16721-16727.	1.1	548
28	Ab initiostudy of ferroelectric domain walls inPbTiO3. Physical Review B, 2002, 65, .	1.1	471
29	Implementation of ultrasoft pseudopotentials inab initiomolecular dynamics. Physical Review B, 1991, 43, 6796-6799.	1.1	453
30	Phonons and lattice dielectric properties of zirconia. Physical Review B, 2002, 65, .	1.1	440
31	Ab initiocalculation of the anomalous Hall conductivity by Wannier interpolation. Physical Review B, 2006, 74, .	1.1	397
32	A Monte carlo simulated annealing approach to optimization over continuous variables. Journal of Computational Physics, 1984, 56, 259-271.	1.9	389
33	First-Principles Approach to Insulators in Finite Electric Fields. Physical Review Letters, 2002, 89, 117602.	2.9	387
34	Enhancement of ferroelectricity at metalâ€“oxide interfaces. Nature Materials, 2009, 8, 392-397.	13.3	383
35	Evidence for the Tunneling Site on Transition-Metal Oxides: TiO2(110). Physical Review Letters, 1996, 77, 1322-1325.	2.9	365
36	Maximally-localized Wannier functions for disordered systems: Application to amorphous silicon. Solid State Communications, 1998, 107, 7-11.	0.9	363

#	Article	IF	Citations
37	Ab initiomolecular dynamics ford-electron systems: Liquid copper at 1500 K. Physical Review Letters, 1992, 69, 1982-1985.	2.9	346
38	Ensemble Density-Functional Theory forAb InitioMolecular Dynamics of Metals and Finite-Temperature Insulators. Physical Review Letters, 1997, 79, 1337-1340.	2.9	345
39	Competing Structural Instabilities in Cubic Perovskites. Physical Review Letters, 1995, 74, 2587-2590.	2.9	327
40	Extrinsic models for the dielectric response of CaCu3Ti4O12. Journal of Applied Physics, 2003, 94, 3299-3306.	1.1	324
41	Z2Pack: Numerical implementation of hybrid Wannier centers for identifying topological materials. Physical Review B, 2017, 95, .	1.1	322
42	Finite-temperature phase diagram of vicinal Si(100) surfaces. Physical Review Letters, 1990, 64, 2406-2409.	2.9	315
43	Berry-phase theory of proper piezoelectric response. Journal of Physics and Chemistry of Solids, 2000, 61, 147-151.	1.9	309
44	Spectral and Fermi surface properties from Wannier interpolation. Physical Review B, 2007, 75, .	1.1	307
45	Ab initiostudy ofBaTiO3andPbTiO3surfaces in external electric fields. Physical Review B, 2001, 63, .	1.1	304
46	Total energies of diamond (111) surface reconstructions by a linear combination of atomic orbitals method. Physical Review B, 1984, 30, 6118-6130.	1.1	303
47	Orbital Magnetization in Periodic Insulators. Physical Review Letters, 2005, 95, 137205.	2.9	300
48	Elastic stress domains and the herringbone reconstruction on Au(111). Physical Review Letters, 1992, 69, 1564-1567.	2.9	285
49	Ab initiostudy of BaTiO3surfaces. Physical Review B, 1997, 56, 1625-1631.	1.1	268
50	First-principles study of epitaxial strain in perovskites. Physical Review B, 2005, 72, .	1.1	261
51	Metric tensor formulation of strain in density-functional perturbation theory. Physical Review B, 2005, 71, .	1.1	260
52	Negative-curvature fullerene analog ofC60. Physical Review Letters, 1992, 68, 511-513.	2.9	257
53	Effect of quantum fluctuations on structural phase transitions inSrTiO3andBaTiO3. Physical Review B, 1996, 53, 5047-5050.	1.1	251
54	Ab initio study of SrTiO3 surfaces. Surface Science, 1998, 418, 64-70.	0.8	251

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55	Surface doping and stabilization of Si(111) with boron. Physical Review Letters, 1989, 63, 1257-1260.	2.9	241
56	Polarization-Based Calculation of the Dielectric Tensor of Polar Crystals. Physical Review Letters, 1997, 79, 3958-3961.	2.9	236
57	Orbital magnetization in crystalline solids: Multi-band insulators, Chern insulators, and metals. Physical Review B, 2006, 74, .	1.1	218
58	Ab initiostudy of the phase diagram of epitaxialBaTiO3. Physical Review B, 2004, 69, .	1.1	217
59	Adatoms on Si(111) and Ge(111) surfaces. Physical Review B, 1989, 40, 3905-3913.	1.1	216
60	Stability of periodic domain structures in a two-dimensional dipolar model. Physical Review B, 1995, 52, 2177-2183.	1.1	206
61	Topological nodal-line semimetals in alkaline-earth stannides, germanides, and silicides. Physical Review B, 2016, 93, .	1.1	201
62	Generalization of the density-matrix method to a nonorthogonal basis. Physical Review B, 1994, 50, 17611-17614.	1.1	199
63	Importance of Second-Order Piezoelectric Effects in Zinc-Blende Semiconductors. Physical Review Letters, 2006, 96, 187602.	2.9	197
64	Absence of large compressive stress on Si(111). Physical Review Letters, 1987, 59, 1456-1459.	2.9	193
65	Theory of PbTiO3, BaTiO3, and SrTiO3 surfaces. Faraday Discussions, 1999, 114, 395-405.	1.6	190
66	Ab initiostudies on high pressure phases of ice. Physical Review Letters, 1992, 69, 462-465.	2.9	187
67	The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design. Npj Computational Materials, 2020, 6, .	3.5	181
68	Structures of small water clusters using gradient-corrected density functional theory. Chemical Physics Letters, 1993, 207, 208-213.	1.2	179
69	Tunability of the dielectric response of epitaxially strainedSrTiO3from first principles. Physical Review B, 2005, 71, .	1.1	178
70	First-principles investigation of 180Â° domain walls in BaTiO3. Physical Review B, 1996, 53, R5969-R5973.	1.1	177
71	Electric-field induced polarization paths inPb(Zr1â^'xTix)O3alloys. Physical Review B, 2001, 64, .	1.1	175
72	Defects onTiO2(110) surfaces. Physical Review B, 1994, 49, 7709-7715.	1.1	171

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73	Origins of stress on elemental and chemisorbed semiconductor surfaces. Physical Review Letters, 1989, 63, 1404-1407.	2.9	170
74	Accurate calculation of polarization-related quantities in semiconductors. Physical Review B, 2001, 63, .	1.1	168
75	Exponential Decay Properties of Wannier Functions and Related Quantities. Physical Review Letters, 2001, 86, 5341-5344.	2.9	164
76	Intrinsic Piezoelectric Response in Perovskite Alloys: PMN-PT versus PZT. Physical Review Letters, 1999, 83, 1347-1350.	2.9	161
77	First-principles study of(BiScO3)1âˆ'xâˆ'(PbTiO3)xpiezoelectric alloys. Physical Review B, 2003, 67, .	1.1	161
78	Ab initiostudies on the structural and dynamical properties of ice. Physical Review B, 1993, 47, 4863-4872.	1.1	160
79	Structural and dielectric properties of crystalline and amorphous ZrO2. Thin Solid Films, 2005, 486, 125-128.	0.8	160
80	Orbital magnetoelectric coupling in band insulators. Physical Review B, 2010, 81, .	1.1	155
81	Annealing of Heavily Arsenic-Doped Silicon: Electrical Deactivation and a New Defect Complex. Physical Review Letters, 1988, 61, 1282-1285.	2.9	153
82	Phase segregation and work-function variations on metal surfaces: spontaneous formation of periodic domain structures. Surface Science, 1992, 268, L300-L304.	0.8	149
83	Ab initio calculations of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Ba</mml:mi><mml:mi mathvariant="normal">Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Pb</mml:mi><mml:mi mathvariant="normal">Ti</mml:mi><mml:msub><mml:mi m	1.1	149
84	Structural and dielectric properties of amorphousZrO2andHfO2. Physical Review B, 2006, 74, .	1.1	148
85	Suppressed Dependence of Polarization on Epitaxial Strain in Highly Polar Ferroelectrics. Physical Review Letters, 2007, 98, 217602.	2.9	146
86	Spin-phonon coupling effects in transition-metal perovskites: A DFTÂ+Â<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>U</mml:mi></mml:math>and hybrid-functional study. Physical Review B, 2012, 85, .	1.1	145
87	Electric displacement as the fundamental variable in electronic-structure calculations. Nature Physics, 2009, 5, 304-308.	6.5	143
88	Wannier center sheets in topological insulators. Physical Review B, 2014, 89, .	1.1	139
89	Structural, electronic, and dielectric properties of amorphousZrO2fromab initiomolecular dynamics. Physical Review B, 2005, 71, .	1.1	135
90	Effects of linear and nonlinear piezoelectricity on the electronic properties ofInAsâ•GaAsquantum dots. Physical Review B, 2006, 74, .	1.1	135

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91	First-principles calculations of atomic and electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SrTiO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> and (011) surfaces. Physical Review B, 2008, 77, .	1.1	132
92	Compositional Inversion Symmetry Breaking in Ferroelectric Perovskites. Physical Review Letters, 2000, 84, 5636-5639.	2.9	128
93	Period-Doubled Structure for the90Â°Partial Dislocation in Silicon. Physical Review Letters, 1997, 79, 245-248.	2.9	127
94	Effective<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>J</mml:mi><mml:mo mathvariant="bold">=</mml:mo><mml:mn>1</mml:mn><mml:mo>/</mml:mo><mml:mn>2</mml:mn></mml:math>Insulating State in Ruddlesden-Popper Iridates: An<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>LDA</mml:mi><mml:mo mathvariant="bold">+</mml:mo><mml:mi>DMFT</mml:mi></mml:math>Study. Physical Review Letters, 2	2.9	124
95	First-principles study of ferroelectric and antiferrodistortive instabilities in tetragonalSrTiO3. Physical Review B, 2000, 62, 13942-13950.	1.1	123
96	Fermi-surface calculation of the anomalous Hall conductivity. Physical Review B, 2007, 76, .	1.1	123
97	Theory of structural response to macroscopic electric fields in ferroelectric systems. Physical Review B, 2002, 66, .	1.1	115
98	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>Semiconductors as Ferroelectrics. Physical Review Letters, 2012, 109, 167602.	2.9	114
99	Model for the energetics of Si and Ge (111) surfaces. Physical Review B, 1987, 36, 6209-6212.	1.1	113
100	Electromechanical behavior of BaTiO3 from first principles. Applied Physics Letters, 1998, 72, 2981-2983.	1.5	113
101	Properties of a Continuous-Random-Network Model for Amorphous Systems. Physical Review Letters, 1998, 81, 4899-4902.	2.9	113
102	First-Principles Study of the Temperature-Pressure Phase Diagram ofBaTiO3. Physical Review Letters, 2002, 89, 115503.	2.9	106
103	Polarization enhancement in two- and three-component ferroelectric superlattices. Applied Physics Letters, 2005, 87, 102906.	1.5	106
104	Non-hysteretic colossal magnetoelectricity in a collinear antiferromagnet. Nature Communications, 2014, 5, 3201.	5.8	106
105	Surfaces of axion insulators. Physical Review B, 2018, 98, .	1.1	103
106	Band alignment issues related to HfO2âˆ•SiO2âˆ•p-Si gate stacks. Journal of Applied Physics, 2004, 96, 7485-7491.	1.1	102
107	Dichroic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>f</mml:mi></mml:math>-sum rule and the orbital magnetization of crystals. Physical Review B, 2008, 77, .	1.1	102
108	Fast molecular-dynamics simulation for ferroelectric thin-film capacitors using a first-principles effective Hamiltonian. Physical Review B, 2008, 78, .	1.1	100

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109	Chern Insulators from Heavy Atoms on Magnetic Substrates. Physical Review Letters, 2013, 110, 116802.	2.9	99
110	Real-Space Approach to Calculation of Electric Polarization and Dielectric Constants. Physical Review Letters, 1994, 73, 712-715.	2.9	96
111	First-principles based modelling of ferroelectrics. Current Opinion in Solid State and Materials Science, 1997, 2, 701-705.	5.6	96
112	Low-Temperature Properties of Pb(Zr 1âˆ' x Ti x)O 3 Solid Solutions near the Morphotropic Phase Boundary. Ferroelectrics, 2002, 266, 41-56.	0.3	95
113	Anomalous enhancement of tetragonality inPbTiO3induced by negative pressure. Physical Review B, 2003, 68, .	1.1	94
114	Structural, electronic, and dielectric properties of ultrathin zirconia films on silicon. Applied Physics Letters, 2005, 86, 152902.	1.5	94
115	First-principles study of stability and vibrational properties of tetragonalPbTiO3. Physical Review B, 1996, 54, 3817-3824.	1.1	93
116	Structural Properties of Lanthanide and Actinide Compounds within the Plane Wave Pseudopotential Approach. Physical Review Letters, 2000, 85, 5122-5125.	2.9	92
117	Chern-Simons orbital magnetoelectric coupling in generic insulators. Physical Review B, 2011, 83, .	1.1	89
118	Electrostatic Model of Atomic Ordering in Complex Perovskite Alloys. Physical Review Letters, 1998, 81, 1318-1321.	2.9	88
119	Structure and oxidation kinetics of the Si(100)-SiO2interface. Physical Review B, 1999, 59, 10132-10137.	1.1	86
120	Dimerization-Induced Cross-Layer Quasi-Two-Dimensionality in Metallic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow><mml:mi>IrTe</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2014, 112, .	2.9	85
121	Chemical hardness, linear response, and pseudopotential transferability. Physical Review B, 1995, 52, 11793-11804.	1.1	83
122	Composite Weyl nodes stabilized by screw symmetry with and without time-reversal invariance. Physical Review B, 2017, 96, .	1.1	82
123	Correct Implementation of Polarization Constants in Wurtzite Materials and Impact on III-Nitrides. Physical Review X, 2016, 6, .	2.8	81
124	Berry-phase theory of polar discontinuities at oxide-oxide interfaces. Physical Review B, 2009, 80, .	1.1	80
125	Hyperferroelectrics: Proper Ferroelectrics with Persistent Polarization. Physical Review Letters, 2014, 112, 127601.	2.9	76
126	Chiral degeneracies and Fermi-surface Chern numbers in bcc Fe. Physical Review B, 2015, 92, .	1.1	76

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127	Emergence of a Chern-insulating state from a semi-Dirac dispersion. Physical Review B, 2015, 92, .	1.1	76
128	Metal-Insulator Transition and Topological Properties of Pyrochlore Iridates. Physical Review Letters, 2017, 118, 026404.	2.9	74
129	Wannier-based calculation of the orbital magnetization in crystals. Physical Review B, 2012, 85, .	1.1	73
130	First-principles studies on structural properties of Î²-cristobalite. Physical Review Letters, 1993, 70, 2750-2753.	2.9	72
131	Full magnetoelectric response of Cr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<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> from first principles. Physical Review B, 2012, 86, .	1.1	72
132	Theory of defect states in glassy selenium. Physical Review B, 1980, 22, 2927-2939.	1.1	70
133	Theory of defect states in glassyAs2Se3. Physical Review B, 1981, 23, 2596-2606.	1.1	70
134	Structure, Barriers, and Relaxation Mechanisms of Kinks in the 90Â° Partial Dislocation in Silicon. Physical Review Letters, 1996, 77, 1516-1519.	2.9	69
135	Anharmonic self-energies of phonons in silicon. Physical Review B, 1991, 43, 4541-4544.	1.1	68
136	First-principles study of crystalline silica. Physical Review B, 1994, 49, 12528-12534.	1.1	68
137	First-principles theory of structural phase transitions for perovskites: Competing instabilities. Ferroelectrics, 1998, 206, 181-204.	0.3	68
138	A first-principles pseudopotential investigation of ferroelectricity in barium titanate. Ferroelectrics, 1992, 136, 85-94.	0.3	67
139	Anharmonic elastic and phonon properties of Si. Physical Review B, 1989, 40, 5657-5668.	1.1	66
140	Robust <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>A</mml:mi></mml:mrow></mml:math> -Type Order and Spin-Flop Transition on the Surface of the Antiferromagnetic Topological Insulator <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow><mml:mi>MnBi</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></ Physical Review Letters, 2020, 125, 037201.	2.9	66
141	Application of a general self-consistency scheme in the linear combination of atomic orbitals formalism to the electronic and structural properties of Si and W. Physical Review B, 1986, 33, 2455-2464.	1.1	65
142	Ab initiocalculations of the atomic and electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CaTiO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></ and (011) surfaces. Physical Review B, 2008, 78, .	1.1	65
143	Maximally localized Wannier functions for GW quasiparticles. Physical Review B, 2009, 79, .	1.1	61
144	Temperature Effects in the Band Structure of Topological Insulators. Physical Review Letters, 2016, 117, 226801.	2.9	61

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145	Atomic structure of dislocation kinks in silicon. Physical Review B, 1998, 57, 10388-10397.	1.1	60
146	First-principles modeling of ferroelectric capacitors via constrained displacement field calculations. Physical Review B, 2009, 80, .	1.1	60
147	Electric Polarization in a Chern Insulator. Physical Review Letters, 2009, 102, 107603.	2.9	60
148	Si-compatible candidates for high-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î</mml:mi></mml:math>dielectrics with the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>P</mml:mi><mml:mi>b</mml:mi><mml:mi>n</mml:mi><mml:mi>m</mml:mi></mml:mrow></r structure. Physical Review B, 2010, 82, .	1.1	59
149	Effects of disorder on the electronic structure of undoped polyacetylene. Physical Review B, 1980, 22, 3939-3948.	1.1	58
150	Calculation of phonon-phonon interactions and two-phonon bound states on the Si(111):H surface. Physical Review Letters, 1992, 69, 2543-2546.	2.9	58
151	Successive Magnetic-Field-Induced Transitions and Colossal Magnetoelectric Effect in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Ni</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></r Physical Review Letters, 2015, 115, 137201.	2.9	58
152	Structure and apparent topography ofTiO2(110)surfaces. Physical Review B, 1997, 56, 10544-10548.	1.1	57
153	Heterovalent andA-atom effects inA(Bâ€²Bâ€³)O3perovskite alloys. Physical Review B, 1999, 59, 1834-1839.	1.1	57
154	Total energy minimization for diamond (111) surfaces: Support for an undimerizedÏ€-bonded chain reconstruction. Physical Review B, 1984, 29, 7099-7101.	1.1	56
155	Atomistic simulations of the incipient ferroelectricKTaO3. Physical Review B, 2004, 70, .	1.1	56
156	Valence and conduction band offsets of a ZrO2/SiOxNy/n-Si CMOS gate stack: A combined photoemission and inverse photoemission study. Physica Status Solidi (B): Basic Research, 2004, 241, 2246-2252.	0.7	56
157	Dissipation due to a â€˜â€˜valley waveâ€™â€™ channel in the quantum Hall effect of a multivalley semiconductor. Physical Review Letters, 1986, 57, 126-129.	2.9	54
158	A converse approach to the calculation of NMR shielding tensors. Journal of Chemical Physics, 2009, 131, 101101.	1.2	54
159	Mn₂FeWO₆: A New Ni₃TeO₆â€Type Polar and Magnetic Oxide. Advanced Materials, 2015, 27, 2177-2181.	11.1	53
160	Total energies in Se. III. Defects in the glass. Physical Review B, 1983, 27, 6311-6321.	1.1	52
161	Interfacial enhancement of ferroelectricity in CaTiO3/BaTiO3superlattices. Physical Review B, 2011, 83, .	1.1	52
162	Polar and phase domain walls with conducting interfacial states in a Weyl semimetal MoTe2. Nature Communications, 2019, 10, 4211.	5.8	50

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163	Systematic beyond-DFT study of binary transition metal oxides. Npj Computational Materials, 2019, 5, .	3.5	50
164	Core reconstruction of the90Â°partial dislocation in nonpolar semiconductors. Physical Review B, 1998, 58, 12563-12566.	1.1	48
165	Quantitative analysis of the first-principles effective Hamiltonian approach to ferroelectric perovskites. Physical Review B, 2003, 67, .	1.1	48
166	Weyl-mediated helical magnetism in NdAlSi. Nature Materials, 2021, 20, 1650-1656.	13.3	48
167	Chern insulator at a magnetic rocksalt interface. Physical Review B, 2014, 90, .	1.1	47
168	Microscopic theory of spin toroidization in periodic crystals. Physical Review B, 2018, 97, .	1.1	47
169	Wannier-Based Definition of Layer Polarizations in Perovskite Superlattices. Physical Review Letters, 2006, 97, 107602.	2.9	46
170	Polar distortions in hydrogen-bonded organic ferroelectrics. Physical Review B, 2011, 84, .	1.1	45
171	Engineering Weyl Phases and Nonlinear Hall Effects in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">T</mml:mi></mml:mrow><mml:mrow><mml:mi>d</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:m - <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>MoTe</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></	2.9	45
172	Calculation of Phonon-Phonon Interactions and the Absence of Two-Phonon Bound States in Diamond. Physical Review Letters, 1984, 53, 1477-1480.	2.9	44
173	Current-density implementation for calculating flexoelectric coefficients. Physical Review B, 2018, 98, .	1.1	44
174	Mott Metal-Insulator Transitions in Pressurized Layered Trichalcogenides. Physical Review Letters, 2019, 123, 236401.	2.9	44
175	Calculation of Defect States in Amorphous Selenium. Physical Review Letters, 1979, 42, 1012-1015.	2.9	43
176	Theoretical study of the cohesive and structural properties of Mo and W in bcc, fcc, and hcp structures. Physical Review B, 1986, 33, 7941-7946.	1.1	43
177	Intertwined Rashba, Dirac, and Weyl Fermions in Hexagonal Hyperferroelectrics. Physical Review Letters, 2016, 117, 076401.	2.9	42
178	Symmorphic Intersecting Nodal Rings in Semiconducting Layers. Physical Review Letters, 2018, 120, 106403.	2.9	42
179	Nonlocality of Kohn-Sham Exchange-Correlation Fields in Dielectrics. Physical Review Letters, 1997, 79, 3966-3969.	2.9	41
180	Calculation of anharmonic phonon couplings in C, Si, and Ge. Physical Review B, 1986, 33, 8740-8747.	1.1	40

#	Article	IF	Citations
181	First-Principles Modeling of Multiferroic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>R</mml:mi><mml:msub><mml:mi>Mn</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2009, 103, 257201.	2.9	40
182	Adiabatic Pumping of Chern-Simons Axion Coupling. Physical Review Letters, 2015, 114, 096401.	2.9	39
183	Surface theorem for the Chern-Simons axion coupling. Physical Review B, 2017, 95, .	1.1	39
184	Structural excitation energies in selenium. Solid State Communications, 1980, 35, 535-538.	0.9	37
185	Finite-temperature properties of disordered and ordered Pb(Sc0.5Nb0.5)O3 alloys. Applied Physics Letters, 2000, 77, 3642-3644.	1.5	37
186	Flux States and Topological Phases from Spontaneous Time-Reversal Symmetry Breaking in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>CrSi</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mi>Ge</mml:mi><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 532 Td (stretchy="false">)</mml:m	2.9	37
187	Systems. Physical Review Letters, 2016, 117, 257201. Elastic Energies of Coherent Germanium Islands on Silicon. Materials Research Society Symposia Proceedings, 1990, 202, 555.	0.1	36
188	Total energies in Se. I. The trigonal crystal. Physical Review B, 1983, 27, 6296-6301.	1.1	35
189	Canonical magnetic insulators with isotropic magnetoelectric coupling. Physical Review B, 2013, 88, .	1.1	34
190	Bond relaxation in Hg1â^'xCdxTe and related alloys. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1987, 5, 3019-3023.	0.9	33
191	Interfacial charge-transfer Mott state in iridateâ€“nickelate superlattices. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 19863-19868.	3.3	31
192	Bonding Coordination Defect ing-Se: A "Positive-U" System. Physical Review Letters, 1982, 49, 823-826.	2.9	30
193	Ab initiostudy of the nonlinear optics of III-V semiconductors in the terahertz regime. Physical Review B, 2006, 74, .	1.1	30
194	Quantum anomalous Hall phase in (001) double-perovskite monolayers via intersite spin-orbit coupling. Physical Review B, 2014, 90, .	1.1	30
195	Antiferroelectric Topological Insulators in Orthorhombic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>A</mml:mi><mml:mi>MgBi</mml:mi></mml:mrow></mml:math> Compounds (<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML") Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 172 Td	2.9	30
196	Semiconductor effective charges from tight-binding theory. Physical Review B, 1996, 53, 15417-15420.	1.1	29
197	Orbital Magnetization in Extended Systems. ChemPhysChem, 2005, 6, 1815-1819.	1.0	28
198	A new iterative scheme for obtaining eigenvectors of large, real-symmetric matrices. Journal of Computational Physics, 1989, 82, 218-228.	1.9	27

#	Article	IF	Citations
199	Interplay of epitaxial strain and rotations in PbTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub><mml:mo>/</mml:mo></mml:mrow></mml:math>PbZrO<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>superlattices from first principles. Physical Review B,	1.1	27
200	Surface polarization and edge charges. Physical Review B, 2015, 92, .	1.1	26
201	Tracking the continuous spin-flop transition in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ni</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> infrared spectroscopy. Physical Review B, 2015, 92, .	1.1	26
202	Magnetoelectric Coupling through the Spin Flop Transition in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Ni</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow> Physical Review Letters, 2016, 117, 147402.	2.9	26
203	Piezochromism in the magnetic chalcogenide MnPS3. Npj Quantum Materials, 2020, 5, .	1.8	26
204	Optical spectroscopy and band gap analysis of hybrid improper ferroelectric Ca3Ti2O7. Applied Physics Letters, 2016, 108, .	1.5	25
205	Axion coupling in the hybrid Wannier representation. Physical Review B, 2020, 101, .	1.1	25
206	First-principles study of antisite and interstitial phosphorus impurities in ZnSe. Physical Review B, 1994, 50, 2711-2714.	1.1	24
207	Structure and energetics of a ferroelectric organic crystal of phenazine and chloranilic acid. Physical Review B, 2012, 86, .	1.1	24
208	Nonreciprocal directional dichroism of a chiral magnet in the visible range. Npj Quantum Materials, 2020, 5, .	1.8	24
209	Temperature dependence of the bulk Rashba splitting in the bismuth tellurohalides. Physical Review Materials, 2017, 1, .	0.9	24
210	Vibrational fingerprints of ferroelectric HfO2. Npj Quantum Materials, 2022, 7, .	1.8	24
211	Total energy method for solids and solid surfaces. International Journal of Quantum Chemistry, 1984, 26, 105-120.	1.0	23
212	Alerhandet al. Reply. Physical Review Letters, 1991, 66, 962-962.	2.9	23
213	Proton transfer in ice. Chemical Physics Letters, 1993, 210, 279-284.	1.2	22
214	Column-V acceptors in ZnSe. Physical Review B, 1993, 48, 17827-17834.	1.1	22
215	Energetics of antiphase boundaries in GaAs. Physical Review B, 1992, 45, 11192-11201.	1.1	21
216	Tunable inverse topological heterostructure utilizing<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mm	1.1	21

#	Article	IF	Citations
217	Geometric and nongeometric contributions to the surface anomalous Hall conductivity. Physical Review B, 2018, 98, .	1.1	21
218	Hydrogen, Acceptors, and H-Acceptor Complexes in GaN. Materials Research Society Symposia Proceedings, 1995, 395, 503.	0.1	20
219	Theoretical phase diagram of ultrathin films of incipient ferroelectrics. Applied Physics Letters, 2007, 90, 242918.	1.5	20
220	Spin-orbit spillage as a measure of band inversion in insulators. Physical Review B, 2014, 90, .	1.1	19
221	Gauge-discontinuity contributions to Chern-Simons orbital magnetoelectric coupling. Physical Review B, 2015, 92, .	1.1	19
222	Trimer bonding states on the surface of the transition-metal dichalcogenide <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>TaT</mml:mi><mml:msub><mml:mi mathvariant="normal">e</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2018, 98, .	1.1	19
223	Designing Multifunctionality via Assembling Dissimilar Materials: Epitaxial AlN/ScN Superlattices. Physical Review Letters, 2019, 123, 096801.	2.9	19
224	Structural and electronic properties of sodium metasilicate. Chemical Physics Letters, 1993, 215, 401-404.	1.2	18
225	Wannier-function description of the electronic polarization and infrared absorption of high-pressure hydrogen. Physical Review B, 2000, 62, 15505-15520.	1.1	18
226	First-Principles Theory of Polarization and Electric Fields in Ferroelectrics. Ferroelectrics, 2004, 301, 9-14.	0.3	18
227	Calculation of C1score-level shifts in poly(ethylene terephthalate) and comparison with x-ray photoelectron spectroscopy. Physical Review B, 2000, 61, 7716-7721.	1.1	17
228	Quadrupole moments, edge polarizations, and corner charges in the Wannier representation. Physical Review B, 2021, 103, .	1.1	17
229	Controllable quantum point junction on the surface of an antiferromagnetic topological insulator. Nature Communications, 2021, 12, 3998.	5.8	17
230	Coulomb interaction and ferroelectric phase transitions in perovskite compounds. Ferroelectrics, 1995, 164, 291-301.	0.3	16
231	Electrically driven octahedral rotations in SrTiO3and PbTiO3. Physical Review B, 2013, 87, .	1.1	16
232	Symmetry crossover in layered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>M</mml:mi><mml:msub><mml:mi>PS</mml:mi><mml:m complexes <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mo>(</mml:mo><mml:mi>M</mml:mi><mml:mo>=</mml:mo><mml:mi>M via near-field infrared spectros. Physical Review B, 2020, 102, .	1.1	16
233	Nexus networks in carbon honeycombs. Physical Review Materials, 2018, 2, .	0.9	16
234	Comment on â€˜â€˜Should all surfaces be reconstructed?â€™â€™. Physical Review Letters, 1993, 71, 461-461.	2.9	15

#	Article	IF	Citations
235	First-principles study of steps on the Si(111):H surface. Physical Review B, 1994, 50, 4637-4641.	1.1	15
236	Generalized-gradient-functional treatment of strain in density-functional perturbation theory. Physical Review B, 2005, 72, .	1.1	15
237	First-principles perturbative computation of phonon properties of insulators in finite electric fields. Physical Review B, 2006, 74, .	1.1	15
238	Covalency-driven collapse of strong spin-orbit coupling in face-sharing iridium octahedra. Physical Review B, 2018, 98, .	1.1	15
239	Near-field infrared spectroscopy of monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">MnPS</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2019, 100, .	1.1	15
240	Metric wave approach to flexoelectricity within density functional perturbation theory. Physical Review B, 2019, 99, .	1.1	15
241	First-principles modeling of strain in perovskite ferroelectric thin films. Phase Transitions, 2008, 81, 607-622.	0.6	14
242	Domain walls and ferroelectric reversal in corundum derivatives. Physical Review B, 2017, 95, .	1.1	14
243	Vibrational properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>CuInP</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>6</mml:mn></mml:mrow></mml:math> across the ferroelectric transition. Physical Review B, 2022, 105, .	1.1	14
244	First-principles study of phosphorus and nitrogen impurities in ZnSe. Physical Review B, 1995, 52, 11912-11919.	1.1	13
245	First-principles theory of magnetically induced ferroelectricity in TbMnO3. European Physical Journal B, 2009, 71, 345-348.	0.6	13
246	Ferromagnetic Anomalous Hall Effect in Cr-Doped Bi2Se3 Thin Films via Surface-State Engineering. Nano Letters, 2019, 19, 3409-3414.	4.5	13
247	Influence of magnetic ordering on the spectral properties of binary transition metal oxides. Physical Review B, 2019, 100, .	1.1	13
248	Total energies in Se. II. Vacancy in the crystal. Physical Review B, 1983, 27, 6302-6310.	1.1	12
249	Chapter 5 Quantum Electrostatics of Insulators: Polarization, Wannier Functions, and Electric Fields. Contemporary Concepts of Condensed Matter Science, 2006, 2, 139-163.	0.5	12
250	Electric field dependence of optical phonon frequencies in wurtzite GaN observed in GaN high electron mobility transistors. Journal of Applied Physics, 2016, 120, .	1.1	12
251	Molecular Mott state in the deficient spinel GaV4S8. Physical Review B, 2020, 102, .	1.1	12
252	First-principles study of high-field piezoelectricity in tetragonalPbTiO3. Physical Review B, 2010, 81, .	1.1	11

#	Article	IF	Citations
253	Quantum theory of mechanical deformations. Physical Review B, 2018, 98, .	1.1	11
254	High-temperature phonon-mediated superconductivity in monolayer Mg2B4C2. Npj Quantum Materials, 2022, 7, .	1.8	11
255	Engineering magnetic topological insulators in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mi>Eu</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math> Zintl compounds. Physical Review B, 2022, 105, .	1.1	11
256	Liuet al. reply. Physical Review Letters, 1993, 71, 3611-3611.	2.9	10
257	ORDERING AT SURFACES FROM ELASTIC AND ELECTROSTATIC INTERACTIONS. Surface Review and Letters, 1997, 04, 811-816.	0.5	10
258	Emergent Magnetic State in (111)-Oriented Quasi-Two-Dimensional Spinel Oxides. Nano Letters, 2019, 19, 8381-8387.	4.5	10
259	Magnetic phase transitions and spin density distribution in the molecular multiferroic system GaV4S8. Physical Review B, 2020, 102, .	1.1	10
260	Exploring few and single layer CrPS₄ with near-field infrared spectroscopy. 2D Materials, 2021, 8, 035020.	2.0	10
261	Structural and Electronic Properties of AlN, GaN And InN, and Band Offsets at AlN/GaN (10<ovl>1</ovl>0) and (0001) Interfaces. Materials Research Society Symposia Proceedings, 1995, 395, 515.	0.1	9
262	Models of core reconstruction for the 90Â° partial dislocation in semiconductors. Journal of Physics Condensed Matter, 2000, 12, 10021-10027.	0.7	9
263	Nature of the magnetic interactions in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sr</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2018, 98, .	1.1	9
264	Lattice dynamics and structural transition of the hyperhoneycomb iridate <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î²</mml:mi><mml:mo>â^’</mml:mo></mml:mrow></mml:math> investigated by high-pressure Raman scattering. Physical Review B, 2020, 101, .	1.1	9
265	Nonreciprocal directional dichroism at telecom wavelengths. Npj Quantum Materials, 2022, 7, .	1.8	9
266	Spontaneous Formation of Stress Domains on Crystal Surfaces. Physical Review Letters, 1989, 62, 116-116.	2.9	8
267	Offsets and Polarization at Strained AlN/GaN Polar Interfaces. Materials Research Society Symposia Proceedings, 1996, 449, 923.	0.1	8
268	Stability of the Period-Doubled Core of the90Â°Partial in Silicon. Physical Review Letters, 2000, 85, 3540-3540.	2.9	8
269	Band-Mott mixing hybridizes the gap in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> <mml:math mathvariant="normal">O</mml:mi><mml:mn>8</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2021, 104, .	1.1	8
270	Total energies of structural defects in glassy Se. Journal of Non-Crystalline Solids, 1983, 59-60, 937-944.	1.5	7

#	Article	IF	Citations
271	Pseudopotential total-energy calculations of column-V acceptors in ZnSe. Physica B: Condensed Matter, 1993, 185, 154-158.	1.3	7
272	Hardness conservation as a new transferability criterion: Application to fully nonlocal pseudopotentials. International Journal of Quantum Chemistry, 1997, 61, 421-427.	1.0	7
273	Gapless hinge states from adiabatic pumping of axion coupling. Physical Review B, 2020, 102, .	1.1	7
274	Lattice dynamics and magnetic exchange interactions in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>GeCo</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> : A spinel with <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>S</mml:mi><mml:mo>=</mml:mo><mml:mfrac><mml:m pyrochlore lattice. Physical Review B, 2021, 104, .	1.1	7
275	Importance of dynamic lattice effects for crystal field excitations in the quantum spin ice candidate <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Pr</mml:mi></mml:mrow><mml:mn>2</mml:mn> mathvariant="normal">O</mml:mi></mml:mrow><mml:mn>7</mml:mn></mml:msub></mml:math>. Physical Review B, 2021, 104, .	1.1	7
276	Maximally-localized Wannier functions in perovskites: Cubic BaTiO[sub 3]. AIP Conference Proceedings, 1998, , .	0.3	6
277	First-principles Study of Electronic and Dielectric Properties of ZrO₂ and HfO₂. Materials Research Society Symposia Proceedings, 2002, 745, 721/T5.2.1.	0.1	6
278	Low-Temperature Properties of Pb(Zr 1âˆ' x Ti x)O 3 Solid Solutions near the Morphotropic Phase Boundary. Ferroelectrics, 2002, 266, 377-392.	0.3	5
279	Mesoscopic Ordering from Elastic and Electrostatic Interactions at Surfaces. , 1993, , 1-11.		5
280	Phonon spectrum of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Pr</mml:mi><mml:mn>2</mml:mn></mml:n mathvariant="normal">O</mml:mi><mml:mn>7</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Pr</mml:mi><mml:mn>2</mml:mn></mml:n m. Physical Review B, 2022, 105, .	1.1	5
281	Off-diagonal occupation numbers in local-density theory. Physical Review B, 1982, 26, 3203-3210.	1.1	4
282	Berry flux diagonalization: Application to electric polarization. Physical Review B, 2020, 102, .	1.1	4
283	Proximate Quantum Spin Liquid on Designer Lattice. Nano Letters, 2021, 21, 2010-2017.	4.5	4
284	Orbital-selective Mott phase and non-Fermi liquid in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>FePS</mml:mi></mml:mrow><mml:mn>3</m Physical Review B, 2022, 105, .	1.1	4
285	Unoccupied electronic structure of Al(111). Physical Review B, 1994, 50, 12025-12032.	1.1	3
286	Ferroelectric and piezoelectric properties in the presence of compositionally broken inversion symmetry. AIP Conference Proceedings, 2001, , .	0.3	3
287	First Principles Calculations of Surface Stress. Materials Research Society Symposia Proceedings, 1988, 141, 451.	0.1	2
288	First-principles Study of Electronic and Dielectric Properties of ZrO2 and HfO2. Materials Research Society Symposia Proceedings, 2002, 747, 1.	0.1	2

#	Article	IF	Citations
289	First-Principles Theory of Flexoelectricity. , 2016, , 31-110.		2
290	Comparison of electromechanical properties of BaTiO[sub 3] between LAPW and a model Hamiltonian. AIP Conference Proceedings, 2000, , .	0.3	1
291	Finite-temperature investigation of ferroelectric solid solutions from first-principles: Application to the structural properties of Pb(Zr[sub 0.5]Ti[sub 0.5])O[sub 3]. AIP Conference Proceedings, 2000, , .	0.3	1
292	Mirror Chern numbers in the hybrid Wannier representation. Physical Review B, 2021, 103, .	1.1	1
293	Polarization Selectivity of Aloof-Beam Electron Energy-Loss Spectroscopy in One-Dimensional ZnO Nanorods. Physical Review Applied, 2021, 16, .	1.5	1
294	Linear phonon-strain coupling in structural phase transitions: Stability of tetragonal PbTiO3. Ferroelectrics, 1997, 194, 29-38.	0.3	0
295	Effective-Hamiltonian Modeling of External Pressures in Ferroelectric Perovskites. AIP Conference Proceedings, 2002, , .	0.3	0
296	A new planar defect in SiGe nanopillars. Microscopy and Microanalysis, 2021, 27, 1948-1949.	0.2	0
297	Origins and Consequences of Surface Stress. Kluwer International Series in Engineering and Computer Science, 1996, , 251-259.	0.2	0