David Vanderbilt

List of Publications by Year in Descending Order

287 papers	63,681 citations	99 h-index	252 g-index
301 ext. papers	70,622 ext. citations	5 avg, IF	8.25 L-index

#	Paper	IF	Citations
287	Nonreciprocal directional dichroism at telecom wavelengths. *Npj Quantum Materials*, **2022**, 7,	5	1
286	Exploring few and single layer CrPS4 with near-field infrared spectroscopy. *2D Materials*, **2021**, 8, 035020	6.9	4
285	Controllable quantum point junction on the surface of an antiferromagnetic topological insulator. *Nature Communications*, **2021**, 12, 3998	17.4	2
284	A new planar defect in SiGe nanopillars. *Microscopy and Microanalysis*, **2021**, 27, 1948-1949	0.5	
283	Lattice dynamics and magnetic exchange interactions in GeCo2O4: A spinel with S=12 pyrochlore lattice. *Physical Review B*, **2021**, 104,	3.3	1
282	Quadrupole moments, edge polarizations, and corner charges in the Wannier representation. *Physical Review B*, **2021**, 103,	3.3	4
281	Proximate Quantum Spin Liquid on Designer Lattice. *Nano Letters*, **2021**, 21, 2010-2017	11.5	2
280	Weyl-mediated helical magnetism in NdAlSi. *Nature Materials*, **2021**, 20, 1650-1656	27	5
279	Molecular Mott state in the deficient spinel GaV4S8. *Physical Review B*, **2020**, 102,	3.3	8
278	Nonreciprocal directional dichroism of a chiral magnet in the visible range. *Npj Quantum Materials*, **2020**, 5,	5	10
277	Magnetic phase transitions and spin density distribution in the molecular multiferroic system GaV4S8. *Physical Review B*, **2020**, 102,	3.3	4
276	Lattice dynamics and structural transition of the hyperhoneycomb iridate □i2IrO3 investigated by high-pressure Raman scattering. *Physical Review B*, **2020**, 101,	3.3	4
275	Axion coupling in the hybrid Wannier representation. *Physical Review B*, **2020**, 101,	3.3	13
274	Wannier90 as a community code: new features and applications. *Journal of Physics Condensed Matter*, **2020**, 32, 165902	1.8	239
273	Engineering Weyl Phases and Nonlinear Hall Effects in T_{d}-MoTe_{2}. *Physical Review Letters*, **2020**, 125, 046402	7.4	12
272	Robust A-Type Order and Spin-Flop Transition on the Surface of the Antiferromagnetic Topological Insulator MnBi_{2}Te_{4}. *Physical Review Letters*, **2020**, 125, 037201	7.4	25
271	The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design. *Npj Computational Materials*, **2020**, 6,	10.9	51

270	Symmetry crossover in layered MPS3 complexes (M=Mn, Fe, Ni) via near-field infrared spectroscopy. *Physical Review B*, **2020**, 102,	3.3	4
269	Berry flux diagonalization: Application to electric polarization. *Physical Review B*, **2020**, 102,	3.3	3
268	Gapless hinge states from adiabatic pumping of axion coupling. *Physical Review B*, **2020**, 102,	3.3	5
267	Piezochromism in the magnetic chalcogenide MnPS3. *Npj Quantum Materials*, **2020**, 5,	5	4
266	Designing Multifunctionality via Assembling Dissimilar Materials: Epitaxial AlN/ScN Superlattices. *Physical Review Letters*, **2019**, 123, 096801	7.4	7
265	Near-field infrared spectroscopy of monolayer MnPS3. *Physical Review B*, **2019**, 100,	3.3	10
264	Polar and phase domain walls with conducting interfacial states in a Weyl semimetal MoTe. *Nature Communications*, **2019**, 10, 4211	17.4	25
263	Interfacial charge-transfer Mott state in iridate-nickelate superlattices. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 19863-19868	11.5	17
262	Metric wave approach to flexoelectricity within density functional perturbation theory. *Physical Review B*, **2019**, 99,	3.3	11
261	Ferromagnetic Anomalous Hall Effect in Cr-Doped BiSe Thin Films via Surface-State Engineering. *Nano Letters*, **2019**, 19, 3409-3414	11.5	7
260	Emergent Magnetic State in (111)-Oriented Quasi-Two-Dimensional Spinel Oxides. *Nano Letters*, **2019**, 19, 8381-8387	11.5	6
259	Systematic beyond-DFT study of binary transition metal oxides. *Npj Computational Materials*, **2019**, 5,	10.9	22
258	Influence of magnetic ordering on the spectral properties of binary transition metal oxides. *Physical Review B*, **2019**, 100,	3.3	8
257	Mott Metal-Insulator Transitions in Pressurized Layered Trichalcogenides. *Physical Review Letters*, **2019**, 123, 236401	7.4	16
256	Symmorphic Intersecting Nodal Rings in Semiconducting Layers. *Physical Review Letters*, **2018**, 120, 106403	7.4	31
255	Microscopic theory of spin toroidization in periodic crystals. *Physical Review B*, **2018**, 97,	3.3	26
254	Nexus networks in carbon honeycombs. *Physical Review Materials*, **2018**, 2,	3.2	13
253	Berry Phases in Electronic Structure Theory: Electric Polarization, Orbital Magnetization and Topological Insulators **2018**,		180

252	Trimer bonding states on the surface of the transition-metal dichalcogenide TaTe2. *Physical Review B*, **2018**, 98,	3.3	8
251	Covalency-driven collapse of strong spin-orbit coupling in face-sharing iridium octahedra. *Physical Review B*, **2018**, 98,	3.3	10
250	Surfaces of axion insulators. *Physical Review B*, **2018**, 98,	3.3	56
249	Nature of the magnetic interactions in Sr3NiIrO6. *Physical Review B*, **2018**, 98,	3.3	4
248	Geometric and nongeometric contributions to the surface anomalous Hall conductivity. *Physical Review B*, **2018**, 98,	3.3	10
247	Quantum theory of mechanical deformations. *Physical Review B*, **2018**, 98,	3.3	8
246	Current-density implementation for calculating flexoelectric coefficients. *Physical Review B*, **2018**, 98,	3.3	26
245	Domain walls and ferroelectric reversal in corundum derivatives. *Physical Review B*, **2017**, 95,	3.3	12
244	Metal-Insulator Transition and Topological Properties of Pyrochlore Iridates. *Physical Review Letters* , **2017**, 118, 026404	7.4	50
243	Z2Pack: Numerical implementation of hybrid Wannier centers for identifying topological materials. *Physical Review B*, **2017**, 95,	3.3	230
242	Surface theorem for the Chern-Simons axion coupling. *Physical Review B*, **2017**, 95,	3.3	26
241	Antiferroelectric Topological Insulators in Orthorhombic AMgBi Compounds (A=Li, Na, K). *Physical Review Letters*, **2017**, 119, 036802	7.4	20
240	Composite Weyl nodes stabilized by screw symmetry with and without time-reversal invariance. *Physical Review B*, **2017**, 96,	3.3	53
239	Temperature dependence of the bulk Rashba splitting in the bismuth tellurohalides. *Physical Review Materials*, **2017**, 1,	3.2	18
238	Temperature Effects in the Band Structure of Topological Insulators. *Physical Review Letters*, **2016**, 117, 226801	7.4	45
237	Tunable inverse topological heterostructure utilizing (Bi1⊠Inx)2Se3 and multichannel weak-antilocalization effect. *Physical Review B*, **2016**, 93,	3.3	19
236	Topological nodal-line semimetals in alkaline-earth stannides, germanides, and silicides. *Physical Review B*, **2016**, 93,	3.3	160
235	Correct Implementation of Polarization Constants in Wurtzite Materials and Impact on III-Nitrides. *Physical Review X*, **2016**, 6,	9.1	49

234	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
233	Electric field dependence of optical phonon frequencies in wurtzite GaN observed in GaN high electron mobility transistors. *Journal of Applied Physics*, **2016**, 120, 155104	2.5	8
232	Flux States and Topological Phases from Spontaneous Time-Reversal Symmetry Breaking in CrSi(Ge)Te_{3}-Based Systems. *Physical Review Letters*, **2016**, 117, 257201	7.4	30
231	Optical spectroscopy and band gap analysis of hybrid improper ferroelectric Ca3Ti2O7. *Applied Physics Letters*, **2016**, 108, 262901	3.4	19
230	Magnetoelectric Coupling through the Spin Flop Transition in Ni_{3}TeO_{6}. *Physical Review Letters* , **2016**, 117, 147402	7.4	15
229	First-Principles Theory of Flexoelectricity **2016**, 31-110		2
228	Intertwined Rashba, Dirac, and Weyl Fermions in Hexagonal Hyperferroelectrics. *Physical Review Letters*, **2016**, 117, 076401	7.4	35
227	Mn2FeWO6 : A new Ni3TeO6-type polar and magnetic oxide. *Advanced Materials*, **2015**, 27, 2177-81	24	43
226	Adiabatic pumping of Chern-Simons axion coupling. *Physical Review Letters*, **2015**, 114, 096401	7.4	29
225	Surface polarization and edge charges. *Physical Review B*, **2015**, 92,	3.3	18
224	Chiral degeneracies and Fermi-surface Chern numbers in bcc Fe. *Physical Review B*, **2015**, 92,	3.3	56
223	Tracking the continuous spin-flop transition in Ni3TeO6 by infrared spectroscopy. *Physical Review B* , **2015**, 92,	3.3	19
222	Emergence of a Chern-insulating state from a semi-Dirac dispersion. *Physical Review B*, **2015**, 92,	3.3	45
221	Gauge-discontinuity contributions to Chern-Simons orbital magnetoelectric coupling. *Physical Review B*, **2015**, 92,	3.3	13
220	Successive Magnetic-Field-Induced Transitions and Colossal Magnetoelectric Effect in Ni_{3}TeO_{6}. *Physical Review Letters*, **2015**, 115, 137201	7.4	40
219	Hyperferroelectrics: proper ferroelectrics with persistent polarization. *Physical Review Letters*, **2014**, 112, 127601	7.4	53
218	Pseudopotentials for high-throughput DFT calculations. *Computational Materials Science*, **2014**, 81, 446-452	3.2	739
217	Non-hysteretic colossal magnetoelectricity in a collinear antiferromagnet. *Nature Communications*, **2014**, 5, 3201	17.4	79

216	Spin-orbit spillage as a measure of band inversion in insulators. *Physical Review B*, **2014**, 90,	3.3	15
215	Chern insulator at a magnetic rocksalt interface. *Physical Review B*, **2014**, 90,	3.3	40
214	Dimerization-Induced Cross-Layer Quasi-Two-Dimensionality in Metallic IrTe2. *Physical Review Letters*, **2014**, 112,	7.4	66
213	Wannier center sheets in topological insulators. *Physical Review B*, **2014**, 89,	3.3	111
212	Quantum anomalous Hall phase in (001) double-perovskite monolayers via intersite spin-orbit coupling. *Physical Review B*, **2014**, 90,	3.3	23
211	An updated version of wannier90: A tool for obtaining maximally-localised Wannier functions. *Computer Physics Communications*, **2014**, 185, 2309-2310	4.2	949
210	Canonical magnetic insulators with isotropic magnetoelectric coupling. *Physical Review B*, **2013**, 88,	3.3	28
209	Electrically driven octahedral rotations in SrTiO3 and PbTiO3. *Physical Review B*, **2013**, 87,	3.3	15
208	Chern insulators from heavy atoms on magnetic substrates. *Physical Review Letters*, **2013**, 110, 116802	7.4	88
207	Effective J=1/2 insulating state in Ruddlesden-Popper iridates: an LDA+DMFT study. *Physical Review Letters*, **2013**, 111, 246402	7.4	104
206	Maximally localized Wannier functions: Theory and applications. *Reviews of Modern Physics*, **2012**, 84, 1419-1475	40.5	1475
205	Hexagonal ABC semiconductors as ferroelectrics. *Physical Review Letters*, **2012**, 109, 167602	7.4	89
204	Full magnetoelectric response of Cr2O3 from first principles. *Physical Review B*, **2012**, 86,	3.3	58
203	Spin-phonon coupling effects in transition-metal perovskites: A DFT + U and hybrid-functional study. *Physical Review B*, **2012**, 85,	3.3	126
202	Wannier-based calculation of the orbital magnetization in crystals. *Physical Review B*, **2012**, 85,	3.3	58
201	Structure and energetics of a ferroelectric organic crystal of phenazine and chloranilic acid. *Physical Review B*, **2012**, 86,	3.3	22
200	Interplay of epitaxial strain and rotations in PbTiO3/PbZrO3 superlattices from first principles. *Physical Review B*, **2011**, 84,	3.3	22
199	Polar distortions in hydrogen-bonded organic ferroelectrics. *Physical Review B*, **2011**, 84,	3.3	43

198	Chern-Simons orbital magnetoelectric coupling in generic insulators. *Physical Review B*, **2011**, 83,	3.3	69
197	Interfacial enhancement of ferroelectricity in CaTiO3/BaTiO3 superlattices. *Physical Review B*, **2011**, 83,	3.3	52
196	Si-compatible candidates for high-□dielectrics with the Pbnm perovskite structure. *Physical Review B*, **2010**, 82,	3.3	52
195	First-principles study of high-field piezoelectricity in tetragonal PbTiO3. *Physical Review B*, **2010**, 81,	3.3	9
194	Orbital magnetoelectric coupling in band insulators. *Physical Review B*, **2010**, 81,	3.3	131
193	Maximally localized Wannier functions for GW quasiparticles. *Physical Review B*, **2009**, 79,	3.3	57
192	First-principles modeling of ferroelectric capacitors via constrained displacement field calculations. *Physical Review B*, **2009**, 80,	3.3	57
191	First-principles modeling of multiferroic RMn2O5. *Physical Review Letters*, **2009**, 103, 257201	7.4	33
190	Berry-phase theory of polar discontinuities at oxide-oxide interfaces. *Physical Review B*, **2009**, 80,	3.3	73
189	Enhancement of ferroelectricity at metal-oxide interfaces. *Nature Materials*, **2009**, 8, 392-7	27	354
188	Electric displacement as the fundamental variable in electronic-structure calculations. *Nature Physics*, **2009**, 5, 304-308	16.2	118
187	First-principles theory of magnetically induced ferroelectricity in TbMnO3. *European Physical Journal B*, **2009**, 71, 345-348	1.2	12
186	A converse approach to the calculation of NMR shielding tensors. *Journal of Chemical Physics*, **2009**, 131, 101101	3.9	49
185	Magnetoelectric polarizability and axion electrodynamics in crystalline insulators. *Physical Review Letters*, **2009**, 102, 146805	7.4	616
184	Electric polarization in a Chern insulator. *Physical Review Letters*, **2009**, 102, 107603	7.4	46
183	Fast molecular-dynamics simulation for ferroelectric thin-film capacitors using a first-principles effective Hamiltonian. *Physical Review B*, **2008**, 78,	3.3	83
182	Dichroic f-sum rule and the orbital magnetization of crystals. *Physical Review B*, **2008**, 77,	3.3	73
181	First-principles calculations of atomic and electronic structure of SrTiO3 (001) and (011) surfaces. *Physical Review B*, **2008**, 77,	3.3	120

180	Ab initio calculations of the atomic and electronic structure of CaTiO3 (001) and (011) surfaces. *Physical Review B*, **2008**, 78,	3.3	60
179	First-principles modeling of strain in perovskite ferroelectric thin films. *Phase Transitions*, **2008**, 81, 607-622	1.3	12
178	wannier90: A tool for obtaining maximally-localised Wannier functions. *Computer Physics Communications*, **2008**, 178, 685-699	4.2	2088
177	Spectral and Fermi surface properties from Wannier interpolation. *Physical Review B*, **2007**, 75,	3.3	248
176	Ab initio calculations of BaTiO3 and PbTiO3 (001) and (011) surface structures. *Physical Review B*, **2007**, 76,	3.3	122
175	Suppressed dependence of polarization on epitaxial strain in highly polar ferroelectrics. *Physical Review Letters*, **2007**, 98, 217602	7.4	138
174	Theoretical phase diagram of ultrathin films of incipient ferroelectrics. *Applied Physics Letters*, **2007** , 90, 242918	3.4	18
173	Fermi-surface calculation of the anomalous Hall conductivity. *Physical Review B*, **2007**, 76,	3.3	96
172	First-principles perturbative computation of phonon properties of insulators in finite electric fields. *Physical Review B*, **2006**, 74,	3.3	12
171	Wannier-based definition of layer polarizations in perovskite superlattices. *Physical Review Letters*, **2006**, 97, 107602	7.4	44
170	Ab initio calculation of the anomalous Hall conductivity by Wannier interpolation. *Physical Review B*, **2006**, 74,	3.3	275
169	Orbital magnetization in crystalline solids: Multi-band insulators, Chern insulators, and metals. *Physical Review B*, **2006**, 74,	3.3	168
168	Ab initio study of the nonlinear optics of III-V semiconductors in the terahertz regime. *Physical Review B*, **2006**, 74,	3.3	26
167	Structural and dielectric properties of amorphous ZrO2 and HfO2. *Physical Review B*, **2006**, 74,	3.3	135
166	Effects of linear and nonlinear piezoelectricity on the electronic properties of InAs□aAs quantum dots. *Physical Review B*, **2006**, 74,	3.3	126
165	Chapter 5 Quantum Electrostatics of Insulators: Polarization, Wannier Functions, and Electric Fields. *Contemporary Concepts of Condensed Matter Science*, **2006**, 2, 139-163		9
164	Importance of second-order piezoelectric effects in zinc-blende semiconductors. *Physical Review Letters*, **2006**, 96, 187602	7.4	174
163	Systematic treatment of displacements, strains, and electric fields in density-functional perturbation theory. *Physical Review B*, **2005**, 72,	3.3	489

162	Metric tensor formulation of strain in density-functional perturbation theory. *Physical Review B*, **2005**, 71,	3.3	218
161	Structural, electronic, and dielectric properties of amorphous ZrO2 from ab initio molecular dynamics. *Physical Review B*, **2005**, 71,	3.3	124
160	Generalized-gradient-functional treatment of strain in density-functional perturbation theory. *Physical Review B*, **2005**, 72,	3.3	14
159	Orbital magnetization in periodic insulators. *Physical Review Letters*, **2005**, 95, 137205	7.4	227
158	First-principles study of epitaxial strain in perovskites. *Physical Review B*, **2005**, 72,	3.3	236
157	Structural and dielectric properties of crystalline and amorphous ZrO2. *Thin Solid Films*, **2005**, 486, 125-128	2.1	142
156	Orbital magnetization in extended systems. *ChemPhysChem*, **2005**, 6, 1815-9	3.2	26
155	Polarization enhancement in two- and three-component ferroelectric superlattices. *Applied Physics Letters*, **2005**, 87, 102906	3.4	99
154	Tunability of the dielectric response of epitaxially strained SrTiO3 from first principles. *Physical Review B*, **2005**, 71,	3.3	162
153	Structural, electronic, and dielectric properties of ultrathin zirconia films on silicon. *Applied Physics Letters*, **2005**, 86, 152902	3.4	81
152	Atomistic simulations of the incipient ferroelectric KTaO3. *Physical Review B*, **2004**, 70,	3.3	47
151	Band alignment issues related to HfO2/SiO2/p-Si gate stacks. *Journal of Applied Physics*, **2004**, 96, 7485-7491	2.5	92
150	First-Principles Theory of Polarization and Electric Fields in Ferroelectrics. *Ferroelectrics*, **2004**, 301, 9-14	0.6	15
149	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	1.3	52
148	Ab initio study of the phase diagram of epitaxial BaTiO3. *Physical Review B*, **2004**, 69,	3.3	201
147	Anomalous enhancement of tetragonality in PbTiO3 induced by negative pressure. *Physical Review B*, **2003**, 68,	3.3	83
146	Extrinsic models for the dielectric response of CaCu3Ti4O12. *Journal of Applied Physics*, **2003**, 94, 3299-3306	2.5	295
145	First-principles study of (BiScO3)1−x(PbTiO3)x piezoelectric alloys. *Physical Review B*, **2003**, 67,	3.3	144

144	Quantitative analysis of the first-principles effective Hamiltonian approach to ferroelectric perovskites. *Physical Review B*, **2003**, 67,	3.3	41
143	First-principles study of the temperature-pressure phase diagram of BaTiO3. *Physical Review Letters*, **2002**, 89, 115503	7.4	94
142	Ab initio study of ferroelectric domain walls in PbTiO3. *Physical Review B*, **2002**, 65,	3.3	417
141	First-principles Study of Electronic and Dielectric Properties of ZrO2 and HfO2. *Materials Research Society Symposia Proceedings*, **2002**, 745, 721/T5.2.1		4
140	First-principles Study of Electronic and Dielectric Properties of ZrO2 and HfO2. *Materials Research Society Symposia Proceedings*, **2002**, 747, 1		
139	First-principles approach to insulators in finite electric fields. *Physical Review Letters*, **2002**, 89, 117602	7.4	300
138	Low-Temperature Properties of Pb(Zr 1□x Ti x)O 3 Solid Solutions near the Morphotropic Phase Boundary. *Ferroelectrics*, **2002**, 266, 41-56	0.6	83
137	Low-Temperature Properties of Pb(Zr 1□x Ti x)O 3 Solid Solutions near the Morphotropic Phase Boundary. *Ferroelectrics*, **2002**, 266, 377-392	0.6	3
136	First-principles study of structural, vibrational, and lattice dielectric properties of hafnium oxide. *Physical Review B*, **2002**, 65,	3.3	543
135	Theory of structural response to macroscopic electric fields in ferroelectric systems. *Physical Review B*, **2002**, 66,	3.3	102
134	Phonons and lattice dielectric properties of zirconia. *Physical Review B*, **2002**, 65,	3.3	389
133	Exponential decay properties of Wannier functions and related quantities. *Physical Review Letters*, **2001**, 86, 5341-4	7.4	147
132	Ab initio study of BaTiO3 and PbTiO3 surfaces in external electric fields. *Physical Review B*, **2001**, 63,	3.3	277
131	Electric-field induced polarization paths in Pb(Zr1□Tix)O3 alloys. *Physical Review B*, **2001**, 64,	3.3	160
130	Accurate calculation of polarization-related quantities in semiconductors. *Physical Review B*, **2001**, 63,	3.3	146
129	Maximally localized Wannier functions for entangled energy bands. *Physical Review B*, **2001**, 65,	3.3	1174
128	Ferroelectric and piezoelectric properties in the presence of compositionally broken inversion symmetry. *AIP Conference Proceedings*, **2001**,	0	3
127	Comparison of electromechanical properties of BaTiO3 between LAPW and a model Hamiltonian. *AIP Conference Proceedings*, **2000**,	0	1

126	Berry-phase theory of proper piezoelectric response. *Journal of Physics and Chemistry of Solids*, **2000**, 61, 147-151	3.9	239
125	Models of core reconstruction for the 90□partial dislocation in semiconductors. *Journal of Physics Condensed Matter*, **2000**, 12, 10021-10027	1.8	8
124	Finite-temperature properties of disordered and ordered Pb(Sc0.5Nb0.5)O3 alloys. *Applied Physics Letters*, **2000**, 77, 3642-3644	3.4	37
123	Stability of the period-doubled core of the 90 degrees partial in silicon. *Physical Review Letters*, **2000**, 85, 3540	7.4	8
122	Calculation of C 1s core-level shifts in poly(ethylene terephthalate) and comparison with x-ray photoelectron spectroscopy. *Physical Review B*, **2000**, 61, 7716-7721	3.3	14
121	First-principles study of ferroelectric and antiferrodistortive instabilities in tetragonal SrTiO3. *Physical Review B*, **2000**, 62, 13942-13950	3.3	110
120	Structural properties of lanthanide and actinide compounds within the plane wave pseudopotential approach. *Physical Review Letters*, **2000**, 85, 5122-5	7.4	84
119	Wannier-function description of the electronic polarization and infrared absorption of high-pressure hydrogen. *Physical Review B*, **2000**, 62, 15505-15520	3.3	17
118	Compositional inversion symmetry breaking in ferroelectric perovskites. *Physical Review Letters*, **2000**, 84, 5636-9	7.4	119
117	Finite-temperature properties of Pb(Zr1-xTi(x))O3 alloys from first principles. *Physical Review Letters*, **2000**, 84, 5427-30	7.4	507
116	Virtual crystal approximation revisited: Application to dielectric and piezoelectric properties of perovskites. *Physical Review B*, **2000**, 61, 7877-7882	3.3	463
115	Heterovalent and A-atom effects in A(B?B?)O3 perovskite alloys. *Physical Review B*, **1999**, 59, 1834-1839	3.3	55
114	Theory of PbTiO3, BaTiO3, and SrTiO3 surfaces. *Faraday Discussions*, **1999**, 114, 395-405	3.6	175
113	Structure and oxidation kinetics of the Si(100)-SiO2 interface. *Physical Review B*, **1999**, 59, 10132-10137	3.3	82
112	Intrinsic Piezoelectric Response in Perovskite Alloys: PMN-PT versus PZT. *Physical Review Letters*, **1999**, 83, 1347-1350	7.4	144
111	Thermal Contraction and Disordering of the Al(110) Surface. *Physical Review Letters*, **1999**, 82, 3296-3299	7.4	700
110	Maximally-localized Wannier functions for disordered systems: Application to amorphous silicon. *Solid State Communications*, **1998**, 107, 7-11	1.6	320
109	Ab initio study of SrTiO3 surfaces. *Surface Science*, **1998**, 418, 64-70	1.8	240

108	Electrostatic Model of Atomic Ordering in Complex Perovskite Alloys. *Physical Review Letters*, **1998**, 81, 1318-1321	7.4	82
107	Electromechanical behavior of BaTiO3 from first principles. *Applied Physics Letters*, **1998**, 72, 2981-2983	3.4	101
106	Core reconstruction of the 90° partial dislocation in nonpolar semiconductors. *Physical Review B*, **1998**, 58, 12563-12566	3.3	46
105	Atomic structure of dislocation kinks in silicon. *Physical Review B*, **1998**, 57, 10388-10397	3.3	51
104	Properties of a Continuous-Random-Network Model for Amorphous Systems. *Physical Review Letters*, **1998**, 81, 4899-4902	7.4	94
103	First-principles theory of structural phase transitions for perovskites: Competing instabilities. *Ferroelectrics*, **1998**, 206, 181-204	0.6	59
102	Maximally-localized Wannier functions in perovskites: Cubic BaTiO3 **1998**,		6
101	Period-Doubled Structure for the 90° Partial Dislocation in Silicon. *Physical Review Letters*, **1997**, 79, 245-248	7.4	114
100	Nonlocality of Kohn-Sham Exchange-Correlation Fields in Dielectrics. *Physical Review Letters*, **1997**, 79, 3966-3969	7.4	35
99	ORDERING AT SURFACES FROM ELASTIC AND ELECTROSTATIC INTERACTIONS. *Surface Review and Letters*, **1997**, 04, 811-816	1.1	8
98	Structure and apparent topography of TiO2(110) surfaces. *Physical Review B*, **1997**, 56, 10544-10548	3.3	49
97	Polarization-Based Calculation of the Dielectric Tensor of Polar Crystals. *Physical Review Letters*, **1997**, 79, 3958-3961	7.4	210
96	Ab initio study of BaTiO3 surfaces. *Physical Review B*, **1997**, 56, 1625-1631	3.3	253
95	Linear phonon-strain coupling in structural phase transitions: Stability of tetragonal PbTiO3. *Ferroelectrics*, **1997**, 194, 29-38	0.6	
94	Maximally localized generalized Wannier functions for composite energy bands. *Physical Review B*, **1997**, 56, 12847-12865	3.3	2886
93	First-principles based modelling of ferroelectrics. *Current Opinion in Solid State and Materials Science*, **1997**, 2, 701-705	12	89
92	Ensemble Density-Functional Theory for Ab Initio Molecular Dynamics of Metals and Finite-Temperature Insulators. *Physical Review Letters*, **1997**, 79, 1337-1340	7.4	277
91	Spontaneous polarization and piezoelectric constants of III-V nitrides. *Physical Review B*, **1997**, 56, R10024-R10027	3.3	2329

90	Hardness conservation as a new transferability criterion: Application to fully nonlocal pseudopotentials. *International Journal of Quantum Chemistry*, **1997**, 61, 421-427	2.1	7
89	Evidence for the Tunneling Site on Transition-Metal Oxides: TiO2(110). *Physical Review Letters*, **1996**, 77, 1322-1325	7.4	331
88	First-principles investigation of 180 degrees domain walls in BaTiO3. *Physical Review B*, **1996**, 53, R5969-R5973	3.3	155
87	Effect of quantum fluctuations on structural phase transitions in SrTiO3 and BaTiO3. *Physical Review B*, **1996**, 53, 5047-5050	3.3	225
86	First-principles study of stability and vibrational properties of tetragonal PbTiO3. *Physical Review B*, **1996**, 54, 3817-3824	3.3	85
85	Offsets and Polarization at Strained AlN/GaN Polar Interfaces. *Materials Research Society Symposia Proceedings*, **1996**, 449, 923		7
84	Structure, Barriers, and Relaxation Mechanisms of Kinks in the 90 degrees Partial Dislocation in Silicon. *Physical Review Letters*, **1996**, 77, 1516-1519	7.4	65
83	Semiconductor effective charges from tight-binding theory. *Physical Review B*, **1996**, 53, 15417-15420	3.3	25
82	Origins and Consequences of Surface Stress. *Kluwer International Series in Engineering and Computer Science*, **1996**, 251-259		
81	First-principles study of phosphorus and nitrogen impurities in ZnSe. *Physical Review B*, **1995**, 52, 11912-11919	3.3	12
80	Stability of periodic domain structures in a two-dimensional dipolar model. *Physical Review B*, **1995**, 52, 2177-2183	3.3	193
79	Coulomb interaction and ferroelectric phase transitions in perovskite compounds. *Ferroelectrics*, **1995**, 164, 291-301	0.6	15
78	First-principles theory of ferroelectric phase transitions for perovskites: The case of BaTiO3. *Physical Review B*, **1995**, 52, 6301-6312	3.3	564
77	Chemical hardness, linear response, and pseudopotential transferability. *Physical Review B*, **1995**, 52, 11793-11804	3.3	58
76	Competing structural instabilities in cubic perovskites. *Physical Review Letters*, **1995**, 74, 2587-2590	7.4	285
75	Hydrogen, Acceptors, and H-Acceptor Complexes in GaN. *Materials Research Society Symposia Proceedings*, **1995**, 395, 503		20
74	Structural and Electronic Properties of AlN, GaN And InN, and Band Offsets at AlN/GaN (1010) and (0001) Interfaces. *Materials Research Society Symposia Proceedings*, **1995**, 395, 515		8
73	Generalization of the density-matrix method to a nonorthogonal basis. *Physical Review B*, **1994**, 50, 17611-17614	3.3	165

72	Defects on TiO2 (110) surfaces. *Physical Review B*, **1994**, 49, 7709-7715	3.3	159
71	Unoccupied electronic structure of Al(111). *Physical Review B*, **1994**, 50, 12025-12032	3.3	2
70	Real-space approach to calculation of electric polarization and dielectric constants. *Physical Review Letters*, **1994**, 73, 712-715	7.4	90
69	First-principles study of crystalline silica. *Physical Review B*, **1994**, 49, 12528-12534	3.3	65
68	First-principles study of antisite and interstitial phosphorus impurities in ZnSe. *Physical Review B*, **1994**, 50, 2711-2714	3.3	22
67	First-principles study of steps on the Si(111):H surface. *Physical Review B*, **1994**, 50, 4637-4641	3.3	14
66	Phase transitions in BaTiO3 from first principles. *Physical Review Letters*, **1994**, 73, 1861-1864	7.4	512
65	First-principles investigation of ferroelectricity in perovskite compounds. *Physical Review B*, **1994**, 49, 5828-5844	3.3	568
64	First-principles calculations of the energetics of stoichiometric TiO2 surfaces. *Physical Review B*, **1994**, 49, 16721-16727	3.3	504
63	Giant LO-TO splittings in perovskite ferroelectrics. *Physical Review Letters*, **1994**, 72, 3618-3621	7.4	729
62	Car-Parrinello molecular dynamics with Vanderbilt ultrasoft pseudopotentials. *Physical Review B*, **1993**, 47, 10142-10153	3.3	1181
61	Theory of polarization of crystalline solids. *Physical Review B*, **1993**, 47, 1651-1654	3.3	2719
60	Electric polarization as a bulk quantity and its relation to surface charge. *Physical Review B*, **1993**, 48, 4442-4455	3.3	852
59	First-principles studies on structural properties of beta -cristobalite. *Physical Review Letters*, **1993**, 70, 2750-2753	7.4	68
58	Column-V acceptors in ZnSe. *Physical Review B*, **1993**, 48, 17827-17834	3.3	20
57	Density-matrix electronic-structure method with linear system-size scaling. *Physical Review B*, **1993**, 47, 10891-10894	3.3	584
56	Comment on "Should all surfaces be reconstructed?". *Physical Review Letters*, **1993**, 71, 461	7.4	13
55	Liu et al. reply. *Physical Review Letters*, **1993**, 71, 3611	7.4	9

54	Ab initio studies on the structural and dynamical properties of ice. *Physical Review B*, **1993**, 47, 4863-4873	3.3	149
53	Structural and electronic properties of sodium metasilicate. *Chemical Physics Letters*, **1993**, 215, 401-404	2.5	15
52	Structures of small water clusters using gradient-corrected density functional theory. *Chemical Physics Letters*, **1993**, 207, 208-213	2.5	164
51	Proton transfer in ice. *Chemical Physics Letters*, **1993**, 210, 279-284	2.5	20
50	Pseudopotential total-energy calculations of column-V acceptors in ZnSe. *Physica B: Condensed Matter*, **1993**, 185, 154-158	2.8	7
49	Mesoscopic Ordering from Elastic and Electrostatic Interactions at Surfaces **1993**, 1-11		4
48	Ab initio studies on high pressure phases of ice. *Physical Review Letters*, **1992**, 69, 462-465	7.4	154
47	Elastic stress domains and the herringbone reconstruction on Au(111). *Physical Review Letters*, **1992**, 69, 1564-1567	7.4	266
46	Calculation of phonon-phonon interactions and two-phonon bound states on the Si(111):H surface. *Physical Review Letters*, **1992**, 69, 2543-2546	7.4	54
45	Energetics of antiphase boundaries in GaAs. *Physical Review B*, **1992**, 45, 11192-11201	3.3	19
44	A first-principles pseudopotential investigation of ferroelectricity in barium titanate. *Ferroelectrics*, **1992**, 136, 85-94	0.6	63
43	Negative-curvature fullerene analog of C60. *Physical Review Letters*, **1992**, 68, 511-513	7.4	232
42	Phase segregation and work-function variations on metal surfaces: spontaneous formation of periodic domain structures. *Surface Science*, **1992**, 268, L300-L304	1.8	144
41	Ab initio molecular dynamics for d-electron systems: Liquid copper at 1500 K. *Physical Review Letters*, **1992**, 69, 1982-1985	7.4	333
40	Alerhand et al. Reply. *Physical Review Letters*, **1991**, 66, 962	7.4	21
39	Implementation of ultrasoft pseudopotentials in ab initio molecular dynamics. *Physical Review B*, **1991**, 43, 6796-6799	3.3	382
38	Anharmonic self-energies of phonons in silicon. *Physical Review B*, **1991**, 43, 4541-4544	3.3	55
37	Elastic Energies of Coherent Germanium Islands on Silicon. *Materials Research Society Symposia Proceedings*, **1990**, 202, 555		34

36	Soft self-consistent pseudopotentials in a generalized eigenvalue formalism. *Physical Review B*, **1990**, 41, 7892-7895	3.3	17917
35	Finite-temperature phase diagram of vicinal Si(100) surfaces. *Physical Review Letters*, **1990**, 64, 2406-2409	7.4	290
34	Origins of stress on elemental and chemisorbed semiconductor surfaces. *Physical Review Letters*, **1989**, 63, 1404-1407	7.4	168
33	Adatoms on Si(111) and Ge(111) surfaces. *Physical Review B*, **1989**, 40, 3905-3913	3.3	208
32	Spontaneous Formation of Stress Domains on Crystal Surfaces. *Physical Review Letters*, **1989**, 62, 116-116	7.4	6
31	Surface doping and stabilization of Si(111) with boron. *Physical Review Letters*, **1989**, 63, 1257-1260	7.4	222
30	Anharmonic elastic and phonon properties of Si. *Physical Review B*, **1989**, 40, 5657-5668	3.3	55
29	A new iterative scheme for obtaining eigenvectors of large, real-symmetric matrices. *Journal of Computational Physics*, **1989**, 82, 218-228	4.1	26
28	Annealing of heavily arsenic-doped silicon: Electrical deactivation and a new defect complex. *Physical Review Letters*, **1988**, 61, 1282-1285	7.4	136
27	Spontaneous formation of stress domains on crystal surfaces. *Physical Review Letters*, **1988**, 61, 1973-1976	7.4	633
26	First Principles Calculations of Surface Stress. *Materials Research Society Symposia Proceedings*, **1988**, 141, 451		2
25	Bond relaxation in Hg1−xCdxTe and related alloys. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **1987**, 5, 3019-3023	2.9	25
24	Absence of large compressive stress on Si(111). *Physical Review Letters*, **1987**, 59, 1456-1459	7.4	188
23	Model for the energetics of Si and Ge (111) surfaces. *Physical Review B*, **1987**, 36, 6209-6212	3.3	112
22	Dissipation due to a "valley wave" channel in the quantum Hall effect of a multivalley semiconductor. *Physical Review Letters*, **1986**, 57, 126-129	7.4	49
21	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	3.3	62
20	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	3.3	42
19	Calculation of anharmonic phonon couplings in C, Si, and Ge. *Physical Review B*, **1986**, 33, 8740-8747	3.3	33

18	Optimally smooth norm-conserving pseudopotentials. *Physical Review B*, **1985**, 32, 8412-8415	3.3	628
17	Total energy minimization for diamond (111) surfaces: Support for an undimerized π-bonded chain reconstruction. *Physical Review B*, **1984**, 29, 7099-7101	3.3	55
16	A Monte carlo simulated annealing approach to optimization over continuous variables. *Journal of Computational Physics*, **1984**, 56, 259-271	4.1	322
15	Total energy method for solids and solid surfaces. *International Journal of Quantum Chemistry*, **1984**, 26, 105-120	2.1	20
14	Total energies of diamond (111) surface reconstructions by a linear combination of atomic orbitals method. *Physical Review B*, **1984**, 30, 6118-6130	3.3	250
13	Calculation of Phonon-Phonon Interactions and the Absence of Two-Phonon Bound States in Diamond. *Physical Review Letters*, **1984**, 53, 1477-1480	7.4	42
12	Total energies of structural defects in glassy Se. *Journal of Non-Crystalline Solids*, **1983**, 59-60, 937-944	3.9	6
11	Total energies in Se. III. Defects in the glass. *Physical Review B*, **1983**, 27, 6311-6321	3.3	47
10	Total energies in Se. I. The trigonal crystal. *Physical Review B*, **1983**, 27, 6296-6301	3.3	32
9	Total energies in Se. II. Vacancy in the crystal. *Physical Review B*, **1983**, 27, 6302-6310	3.3	9
8	Bonding Coordination Defect in g-Se: A "Positive-U" System. *Physical Review Letters*, **1982**, 49, 823-826	7.4	28
7	Off-diagonal occupation numbers in local-density theory. *Physical Review B*, **1982**, 26, 3203-3210	3.3	4
6	Theory of defect states in glassy As2Se3. *Physical Review B*, **1981**, 23, 2596-2606	3.3	64
5	Structural excitation energies in selenium. *Solid State Communications*, **1980**, 35, 535-538	1.6	35
4	Effects of disorder on the electronic structure of undoped polyacetylene. *Physical Review B*, **1980**, 22, 3939-3948	3.3	55
3	Theory of defect states in glassy selenium. *Physical Review B*, **1980**, 22, 2927-2939	3.3	62
2	Calculation of Defect States in Amorphous Selenium. *Physical Review Letters*, **1979**, 42, 1012-1015	7.4	42
1	Bonding Coordination Defects in Selenium. *Springer Series in Solid-state Sciences*, **1979**, 203-205	0.4	1