David Vanderbilt

List of Publications by Citations

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	Soft self-consistent pseudopotentials in a generalized eigenvalue formalism. *Physical Review B*, **1990**, 41, 7892-7895	3.3	17917
286	Maximally localized generalized Wannier functions for composite energy bands. *Physical Review B*, **1997**, 56, 12847-12865	3.3	2886
285	Theory of polarization of crystalline solids. *Physical Review B*, **1993**, 47, 1651-1654	3.3	2719
284	Spontaneous polarization and piezoelectric constants of III-V nitrides. *Physical Review B*, **1997**, 56, R10024-R10027	3.3	2329
283	wannier90: A tool for obtaining maximally-localised Wannier functions. *Computer Physics Communications*, **2008**, 178, 685-699	4.2	2088
282	Maximally localized Wannier functions: Theory and applications. *Reviews of Modern Physics*, **2012**, 84, 1419-1475	40.5	1475
281	Car-Parrinello molecular dynamics with Vanderbilt ultrasoft pseudopotentials. *Physical Review B*, **1993**, 47, 10142-10153	3.3	1181
280	Maximally localized Wannier functions for entangled energy bands. *Physical Review B*, **2001**, 65,	3.3	1174
279	An updated version of wannier90: A tool for obtaining maximally-localised Wannier functions. *Computer Physics Communications*, **2014**, 185, 2309-2310	4.2	949
278	Electric polarization as a bulk quantity and its relation to surface charge. *Physical Review B*, **1993**, 48, 4442-4455	3.3	852
277	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
276	Pseudopotentials for high-throughput DFT calculations. *Computational Materials Science*, **2014**, 81, 446-452	3.2	739
275	Giant LO-TO splittings in perovskite ferroelectrics. *Physical Review Letters*, **1994**, 72, 3618-3621	7.4	729
274	Thermal Contraction and Disordering of the Al(110) Surface. *Physical Review Letters*, **1999**, 82, 3296-3299	7.4	700
273	Spontaneous formation of stress domains on crystal surfaces. *Physical Review Letters*, **1988**, 61, 1973-1976	7.4	633
272	Optimally smooth norm-conserving pseudopotentials. *Physical Review B*, **1985**, 32, 8412-8415	3.3	628
271	Magnetoelectric polarizability and axion electrodynamics in crystalline insulators. *Physical Review Letters*, **2009**, 102, 146805	7.4	616

270	Density-matrix electronic-structure method with linear system-size scaling. *Physical Review B*, **1993**, 47, 10891-10894	3.3	584
269	First-principles investigation of ferroelectricity in perovskite compounds. *Physical Review B*, **1994**, 49, 5828-5844	3.3	568
268	First-principles theory of ferroelectric phase transitions for perovskites: The case of BaTiO3. *Physical Review B*, **1995**, 52, 6301-6312	3.3	564
267	First-principles study of structural, vibrational, and lattice dielectric properties of hafnium oxide. *Physical Review B*, **2002**, 65,	3.3	543
266	Phase transitions in BaTiO3 from first principles. *Physical Review Letters*, **1994**, 73, 1861-1864	7.4	512
265	Finite-temperature properties of Pb(Zr1-xTi(x))O3 alloys from first principles. *Physical Review Letters*, **2000**, 84, 5427-30	7.4	507
264	First-principles calculations of the energetics of stoichiometric TiO2 surfaces. *Physical Review B*, **1994**, 49, 16721-16727	3.3	504
263	Systematic treatment of displacements, strains, and electric fields in density-functional perturbation theory. *Physical Review B*, **2005**, 72,	3.3	489
262	Virtual crystal approximation revisited: Application to dielectric and piezoelectric properties of perovskites. *Physical Review B*, **2000**, 61, 7877-7882	3.3	463
261	Ab initio study of ferroelectric domain walls in PbTiO3. *Physical Review B*, **2002**, 65,	3.3	417
260	Phonons and lattice dielectric properties of zirconia. *Physical Review B*, **2002**, 65,	3.3	389
259	Implementation of ultrasoft pseudopotentials in ab initio molecular dynamics. *Physical Review B*, **1991**, 43, 6796-6799	3.3	382
258	Enhancement of ferroelectricity at metal-oxide interfaces. *Nature Materials*, **2009**, 8, 392-7	27	354
257	Ab initio molecular dynamics for d-electron systems: Liquid copper at 1500 K. *Physical Review Letters*, **1992**, 69, 1982-1985	7.4	333
256	Evidence for the Tunneling Site on Transition-Metal Oxides: TiO2(110). *Physical Review Letters*, **1996**, 77, 1322-1325	7.4	331
255	A Monte carlo simulated annealing approach to optimization over continuous variables. *Journal of Computational Physics*, **1984**, 56, 259-271	4.1	322
254	Maximally-localized Wannier functions for disordered systems: Application to amorphous silicon. *Solid State Communications*, **1998**, 107, 7-11	1.6	320
253	First-principles approach to insulators in finite electric fields. *Physical Review Letters*, **2002**, 89, 117602	7.4	300

252	Extrinsic models for the dielectric response of CaCu3Ti4O12. *Journal of Applied Physics*, **2003**, 94, 3299-3306	2.5	295
251	Finite-temperature phase diagram of vicinal Si(100) surfaces. *Physical Review Letters*, **1990**, 64, 2406-2409	7.4	290
250	Competing structural instabilities in cubic perovskites. *Physical Review Letters*, **1995**, 74, 2587-2590	7.4	285
249	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
248	Ab initio study of BaTiO3 and PbTiO3 surfaces in external electric fields. *Physical Review B*, **2001**, 63,	3.3	277
247	Ab initio calculation of the anomalous Hall conductivity by Wannier interpolation. *Physical Review B*, **2006**, 74,	3.3	275
246	Elastic stress domains and the herringbone reconstruction on Au(111). *Physical Review Letters*, **1992**, 69, 1564-1567	7.4	266
245	Ab initio study of BaTiO3 surfaces. *Physical Review B*, **1997**, 56, 1625-1631	3.3	253
244	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
243	Spectral and Fermi surface properties from Wannier interpolation. *Physical Review B*, **2007**, 75,	3.3	248
242	Ab initio study of SrTiO3 surfaces. *Surface Science*, **1998**, 418, 64-70	1.8	240
241	Berry-phase theory of proper piezoelectric response. *Journal of Physics and Chemistry of Solids*, **2000**, 61, 147-151	3.9	239
240	Wannier90 as a community code: new features and applications. *Journal of Physics Condensed Matter*, **2020**, 32, 165902	1.8	239
239	First-principles study of epitaxial strain in perovskites. *Physical Review B*, **2005**, 72,	3.3	236
238	Negative-curvature fullerene analog of C60. *Physical Review Letters*, **1992**, 68, 511-513	7.4	232
237	Z2Pack: Numerical implementation of hybrid Wannier centers for identifying topological materials. *Physical Review B*, **2017**, 95,	3.3	230
236	Orbital magnetization in periodic insulators. *Physical Review Letters*, **2005**, 95, 137205	7.4	227
235	Effect of quantum fluctuations on structural phase transitions in SrTiO3 and BaTiO3. *Physical Review B*, **1996**, 53, 5047-5050	3.3	225

234	Surface doping and stabilization of Si(111) with boron. *Physical Review Letters*, **1989**, 63, 1257-1260	7.4	222
233	Metric tensor formulation of strain in density-functional perturbation theory. *Physical Review B*, **2005**, 71,	3.3	218
232	Polarization-Based Calculation of the Dielectric Tensor of Polar Crystals. *Physical Review Letters*, **1997**, 79, 3958-3961	7.4	210
231	Adatoms on Si(111) and Ge(111) surfaces. *Physical Review B*, **1989**, 40, 3905-3913	3.3	208
230	Ab initio study of the phase diagram of epitaxial BaTiO3. *Physical Review B*, **2004**, 69,	3.3	201
229	Stability of periodic domain structures in a two-dimensional dipolar model. *Physical Review B*, **1995**, 52, 2177-2183	3.3	193
228	Absence of large compressive stress on Si(111). *Physical Review Letters*, **1987**, 59, 1456-1459	7.4	188
227	Berry Phases in Electronic Structure Theory: Electric Polarization, Orbital Magnetization and Topological Insulators **2018**,		180
226	Theory of PbTiO3, BaTiO3, and SrTiO3 surfaces. *Faraday Discussions*, **1999**, 114, 395-405	3.6	175
225	Importance of second-order piezoelectric effects in zinc-blende semiconductors. *Physical Review Letters*, **2006**, 96, 187602	7.4	174
224	Orbital magnetization in crystalline solids: Multi-band insulators, Chern insulators, and metals. *Physical Review B*, **2006**, 74,	3.3	168
223	Origins of stress on elemental and chemisorbed semiconductor surfaces. *Physical Review Letters*, **1989**, 63, 1404-1407	7.4	168
222	Generalization of the density-matrix method to a nonorthogonal basis. *Physical Review B*, **1994**, 50, 17611-17614	3.3	165
221	Structures of small water clusters using gradient-corrected density functional theory. *Chemical Physics Letters*, **1993**, 207, 208-213	2.5	164
220	Tunability of the dielectric response of epitaxially strained SrTiO3 from first principles. *Physical Review B*, **2005**, 71,	3.3	162
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218	Electric-field induced polarization paths in Pb(Zr1−xTix)O3 alloys. *Physical Review B*, **2001**, 64,	3.3	160
217	Defects on TiO2 (110) surfaces. *Physical Review B*, **1994**, 49, 7709-7715	3.3	159

216	First-principles investigation of 180 degrees domain walls in BaTiO3. *Physical Review B*, **1996**, 53, R5969-R5973	3.3	155
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214	Ab initio studies on the structural and dynamical properties of ice. *Physical Review B*, **1993**, 47, 4863-4872	3.3	149
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211	First-principles study of (BiScO3)1−x(PbTiO3)x piezoelectric alloys. *Physical Review B*, **2003**, 67,	3.3	144
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209	Phase segregation and work-function variations on metal surfaces: spontaneous formation of periodic domain structures. *Surface Science*, **1992**, 268, L300-L304	1.8	144
208	Structural and dielectric properties of crystalline and amorphous ZrO2. *Thin Solid Films*, **2005**, 486, 125-128	2.1	142
207	Suppressed dependence of polarization on epitaxial strain in highly polar ferroelectrics. *Physical Review Letters*, **2007**, 98, 217602	7.4	138
206	Annealing of heavily arsenic-doped silicon: Electrical deactivation and a new defect complex. *Physical Review Letters*, **1988**, 61, 1282-1285	7.4	136
205	Structural and dielectric properties of amorphous ZrO2 and HfO2. *Physical Review B*, **2006**, 74,	3.3	135
204	Orbital magnetoelectric coupling in band insulators. *Physical Review B*, **2010**, 81,	3.3	131
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	Effects of linear and nonlinear piezoelectricity on the electronic properties of InAs/GaAs quantum dots. *Physical Review B*, **2006**, 74,	3.3	126
201	Structural, electronic, and dielectric properties of amorphous ZrO2 from ab initio molecular dynamics. *Physical Review B*, **2005**, 71,	3.3	124
200	Ab initio calculations of BaTiO3 and PbTiO3 (001) and (011) surface structures. *Physical Review B*, **2007**, 76,	3.3	122
199	First-principles calculations of atomic and electronic structure of SrTiO3 (001) and (011) surfaces. *Physical Review B*, **2008**, 77,	3.3	120

198	Compositional inversion symmetry breaking in ferroelectric perovskites. *Physical Review Letters*, **2000**, 84, 5636-9	7.4	119
197	Electric displacement as the fundamental variable in electronic-structure calculations. *Nature Physics*, **2009**, 5, 304-308	16.2	118
196	Period-Doubled Structure for the 90° Partial Dislocation in Silicon. *Physical Review Letters*, **1997**, 79, 245-248	7.4	114
195	Model for the energetics of Si and Ge (111) surfaces. *Physical Review B*, **1987**, 36, 6209-6212	3.3	112
194	Wannier center sheets in topological insulators. *Physical Review B*, **2014**, 89,	3.3	111
193	First-principles study of ferroelectric and antiferrodistortive instabilities in tetragonal SrTiO3. *Physical Review B*, **2000**, 62, 13942-13950	3.3	110
192	Effective J=1/2 insulating state in Ruddlesden-Popper iridates: an LDA+DMFT study. *Physical Review Letters*, **2013**, 111, 246402	7.4	104
191	Theory of structural response to macroscopic electric fields in ferroelectric systems. *Physical Review B*, **2002**, 66,	3.3	102
190	Electromechanical behavior of BaTiO3 from first principles. *Applied Physics Letters*, **1998**, 72, 2981-2983	3.4	101
189	Polarization enhancement in two- and three-component ferroelectric superlattices. *Applied Physics Letters*, **2005**, 87, 102906	3.4	99
188	Fermi-surface calculation of the anomalous Hall conductivity. *Physical Review B*, **2007**, 76,	3.3	96
187	First-principles study of the temperature-pressure phase diagram of BaTiO3. *Physical Review Letters*, **2002**, 89, 115503	7.4	94
186	Properties of a Continuous-Random-Network Model for Amorphous Systems. *Physical Review Letters*, **1998**, 81, 4899-4902	7.4	94
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183	Hexagonal ABC semiconductors as ferroelectrics. *Physical Review Letters*, **2012**, 109, 167602	7.4	89
182	First-principles based modelling of ferroelectrics. *Current Opinion in Solid State and Materials Science*, **1997**, 2, 701-705	12	89
181	Chern insulators from heavy atoms on magnetic substrates. *Physical Review Letters*, **2013**, 110, 116802	7.4	88

180	First-principles study of stability and vibrational properties of tetragonal PbTiO3. *Physical Review B*, **1996**, 54, 3817-3824	3.3	85
179	Structural properties of lanthanide and actinide compounds within the plane wave pseudopotential approach. *Physical Review Letters*, **2000**, 85, 5122-5	7.4	84
178	Fast molecular-dynamics simulation for ferroelectric thin-film capacitors using a first-principles effective Hamiltonian. *Physical Review B*, **2008**, 78,	3.3	83
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176	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
175	Electrostatic Model of Atomic Ordering in Complex Perovskite Alloys. *Physical Review Letters*, **1998**, 81, 1318-1321	7.4	82
174	Structure and oxidation kinetics of the Si(100)-SiO2 interface. *Physical Review B*, **1999**, 59, 10132-10137	3.3	82
173	Structural, electronic, and dielectric properties of ultrathin zirconia films on silicon. *Applied Physics Letters*, **2005**, 86, 152902	3.4	81
172	Non-hysteretic colossal magnetoelectricity in a collinear antiferromagnet. *Nature Communications*, **2014**, 5, 3201	17.4	79
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170	Dichroic f-sum rule and the orbital magnetization of crystals. *Physical Review B*, **2008**, 77,	3.3	73
169	Chern-Simons orbital magnetoelectric coupling in generic insulators. *Physical Review B*, **2011**, 83,	3.3	69
168	First-principles studies on structural properties of beta -cristobalite. *Physical Review Letters*, **1993**, 70, 2750-2753	7.4	68
167	Dimerization-Induced Cross-Layer Quasi-Two-Dimensionality in Metallic IrTe2. *Physical Review Letters*, **2014**, 112,	7.4	66
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163	A first-principles pseudopotential investigation of ferroelectricity in barium titanate. *Ferroelectrics*, **1992**, 136, 85-94	0.6	63

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161	Theory of defect states in glassy selenium. *Physical Review B*, **1980**, 22, 2927-2939	3.3	62
160	Ab initio calculations of the atomic and electronic structure of CaTiO3 (001) and (011) surfaces. *Physical Review B*, **2008**, 78,	3.3	60
159	First-principles theory of structural phase transitions for perovskites: Competing instabilities. *Ferroelectrics*, **1998**, 206, 181-204	0.6	59
158	Full magnetoelectric response of Cr2O3 from first principles. *Physical Review B*, **2012**, 86,	3.3	58
157	Wannier-based calculation of the orbital magnetization in crystals. *Physical Review B*, **2012**, 85,	3.3	58
156	Chemical hardness, linear response, and pseudopotential transferability. *Physical Review B*, **1995**, 52, 11793-11804	3.3	58
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149	Anharmonic self-energies of phonons in silicon. *Physical Review B*, **1991**, 43, 4541-4544	3.3	55
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144	Composite Weyl nodes stabilized by screw symmetry with and without time-reversal invariance. *Physical Review B*, **2017**, 96,	3.3	53
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140	Atomic structure of dislocation kinks in silicon. *Physical Review B*, **1998**, 57, 10388-10397	3.3	51
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138	Metal-Insulator Transition and Topological Properties of Pyrochlore Iridates. *Physical Review Letters* , **2017**, 118, 026404	7.4	50
137	Correct Implementation of Polarization Constants in Wurtzite Materials and Impact on III-Nitrides. *Physical Review X*, **2016**, 6,	9.1	49
136	A converse approach to the calculation of NMR shielding tensors. *Journal of Chemical Physics*, **2009**, 131, 101101	3.9	49
135	Structure and apparent topography of TiO2(110) surfaces. *Physical Review B*, **1997**, 56, 10544-10548	3.3	49
134	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
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130	Core reconstruction of the 90□partial dislocation in nonpolar semiconductors. *Physical Review B*, **1998**, 58, 12563-12566	3.3	46
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122	Calculation of Defect States in Amorphous Selenium. *Physical Review Letters*, **1979**, 42, 1012-1015	7.4	42
121	Quantitative analysis of the first-principles effective Hamiltonian approach to ferroelectric perovskites. *Physical Review B*, **2003**, 67,	3.3	41
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95	Quantum anomalous Hall phase in (001) double-perovskite monolayers via intersite spin-orbit coupling. *Physical Review B*, **2014**, 90,	3.3	23
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