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	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</mml:mn></mml:msub></mml:math>. Physical Review B, 2022, 105, .	1.1	4
2	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:msub><mml:msub><mml:mi 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:msub></mml:m. Physical Review B, 2022, 105, .	1.1	5
3	Vibrational fingerprints of ferroelectric HfO2. Npj Quantum Materials, 2022, 7, .	1.8	24
4	Nonreciprocal directional dichroism at telecom wavelengths. Npj Quantum Materials, 2022, 7, .	1.8	9
5	High-temperature phonon-mediated superconductivity in monolayer Mg2B4C2. Npj Quantum Materials, 2022, 7, .	1.8	11
6	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:m mathvariant="normal">S</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:mrow></mml:math> across the ferroelectric transition. Physical Review B, 2022, 105, .	1.1	14
7	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:mn>1</mml:mn></mml:msub><mml:mrow><m Zintl compounds. Physical Review B, 2022, 105, .	1.1	11
8	Quadrupole moments, edge polarizations, and corner charges in the Wannier representation. Physical Review B, 2021, 103, .	1.1	17
9	Proximate Quantum Spin Liquid on Designer Lattice. Nano Letters, 2021, 21, 2010-2017.	4.5	4
10	Exploring few and single layer CrPS₄ with near-field infrared spectroscopy. 2D Materials, 2021, 8, 035020.	2.0	10
11	Mirror Chern numbers in the hybrid Wannier representation. Physical Review B, 2021, 103, .	1.1	1
12	Controllable quantum point junction on the surface of an antiferromagnetic topological insulator. Nature Communications, 2021, 12, 3998.	5.8	17
13	A new planar defect in SiGe nanopillars. Microscopy and Microanalysis, 2021, 27, 1948-1949.	0.2	0
14	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:m 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
15	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></m mathvariant="normal">O</mml:mi></mml:mrow><mml:mn>7</mml:mn></mml:msub></mml:math>. Physical Review B, 2021, 104, .	1.1	7
16	Weyl-mediated helical magnetism in NdAlSi. Nature Materials, 2021, 20, 1650-1656.	13.3	48
17	Polarization Selectivity of Aloof-Beam Electron Energy-Loss Spectroscopy in One-Dimensional ZnO Nanorods. Physical Review Applied, 2021, 16, .	1.5	1
18	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:m mathvariant="normal">O</mml:mi><mml:mn>8</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2021, 104, .	1.1	8

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19	Wannier90 as a community code: new features and applications. Journal of Physics Condensed Matter, 2020, 32, 165902.	0.7	807
20	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:math> Stacked Nonmagnetic Layers. Physical Review Letters, 2020, 125, 196403.	2.9	45
21	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></mml:msub></mml:math>. Physical Review Letters, 2020, 125, 037201.	2.9	66
22	The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design. Npj Computational Materials, 2020, 6, .	3.5	181
23	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>N via near-field infrared spectros. Physical Review B, 2020, 102, .	1.1	16
24	Berry flux diagonalization: Application to electric polarization. Physical Review B, 2020, 102, .	1.1	4
25	Gapless hinge states from adiabatic pumping of axion coupling. Physical Review B, 2020, 102, .	1.1	7
26	Piezochromism in the magnetic chalcogenide MnPS3. Npj Quantum Materials, 2020, 5, .	1.8	26
27	Molecular Mott state in the deficient spinel GaV4S8. Physical Review B, 2020, 102, .	1.1	12
28	Nonreciprocal directional dichroism of a chiral magnet in the visible range. Npj Quantum Materials, 2020, 5, .	1.8	24
29	Magnetic phase transitions and spin density distribution in the molecular multiferroic system GaV4S8. Physical Review B, 2020, 102, .	1.1	10
30	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:mi>Li</mml:mi><mml:msub><mml:m investigated by high-pressure Raman scattering. Physical Review B, 2020, 101, .	1.1	9
31	Axion coupling in the hybrid Wannier representation. Physical Review B, 2020, 101, .	1.1	25
32	Emergent Magnetic State in (111)-Oriented Quasi-Two-Dimensional Spinel Oxides. Nano Letters, 2019, 19, 8381-8387.	4.5	10
33	Designing Multifunctionality via Assembling Dissimilar Materials: Epitaxial AlN/ScN Superlattices. Physical Review Letters, 2019, 123, 096801.	2.9	19
34	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
35	Polar and phase domain walls with conducting interfacial states in a Weyl semimetal MoTe2. Nature Communications, 2019, 10, 4211.	5.8	50
36	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

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37	Metric wave approach to flexoelectricity within density functional perturbation theory. Physical Review B, 2019, 99, .	1.1	15
38	Ferromagnetic Anomalous Hall Effect in Cr-Doped Bi2Se3 Thin Films via Surface-State Engineering. Nano Letters, 2019, 19, 3409-3414.	4.5	13
39	Systematic beyond-DFT study of binary transition metal oxides. Npj Computational Materials, 2019, 5, .	3.5	50
40	Influence of magnetic ordering on the spectral properties of binary transition metal oxides. Physical Review B, 2019, 100, .	1.1	13
41	Mott Metal-Insulator Transitions in Pressurized Layered Trichalcogenides. Physical Review Letters, 2019, 123, 236401.	2.9	44
42	Symmorphic Intersecting Nodal Rings in Semiconducting Layers. Physical Review Letters, 2018, 120, 106403.	2.9	42
43	Microscopic theory of spin toroidization in periodic crystals. Physical Review B, 2018, 97, .	1.1	47
44	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
45	Covalency-driven collapse of strong spin-orbit coupling in face-sharing iridium octahedra. Physical Review B, 2018, 98, .	1.1	15
46	Surfaces of axion insulators. Physical Review B, 2018, 98, .	1.1	103
47	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
48	Geometric and nongeometric contributions to the surface anomalous Hall conductivity. Physical Review B, 2018, 98, .	1.1	21
49	Quantum theory of mechanical deformations. Physical Review B, 2018, 98, .	1.1	11
50	Current-density implementation for calculating flexoelectric coefficients. Physical Review B, 2018, 98, .	1.1	44
51	Nexus networks in carbon honeycombs. Physical Review Materials, 2018, 2, .	0.9	16
52	Domain walls and ferroelectric reversal in corundum derivatives. Physical Review B, 2017, 95, .	1.1	14
53	Metal-Insulator Transition and Topological Properties of Pyrochlore Iridates. Physical Review Letters, 2017, 118, 026404.	2.9	74
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56	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 ETQq0 0 0 rgBT /Overlock 10 Tf 50 692 Td (display=	2.9	30
57	Composite Weyl nodes stabilized by screw symmetry with and without time-reversal invariance. Physical Review B, 2017, 96, .	1.1	82
58	Temperature dependence of the bulk Rashba splitting in the bismuth tellurohalides. Physical Review Materials, 2017, 1, .	0.9	24
59	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
60	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
61	Systems. Physical Review Letters, 2016, 117, 257201. Optical spectroscopy and band gap analysis of hybrid improper ferroelectric Ca3Ti2O7. Applied Physics Letters, 2016, 108, .	1.5	25
62	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:mm Physical Review Letters, 2016, 117, 147402.	2.9	26
63	First-Principles Theory of Flexoelectricity. , 2016, , 31-110.		2
64	Intertwined Rashba, Dirac, and Weyl Fermions in Hexagonal Hyperferroelectrics. Physical Review Letters, 2016, 117, 076401.	2.9	42
65	Temperature Effects in the Band Structure of Topological Insulators. Physical Review Letters, 2016, 117, 226801.	2.9	61
66	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><mml:mm	1.1	21
67	Topological nodal-line semimetals in alkaline-earth stannides, germanides, and silicides. Physical Review B, 2016, 93, .	1.1	201
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69	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
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72	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:m infrared spectroscopy. Physical Review B, 2015, 92, .	1.1	26

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74	Gauge-discontinuity contributions to Chern-Simons orbital magnetoelectric coupling. Physical Review B, 2015, 92, .	1.1	19
75	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></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review Letters, 2015, 115, 137201.	2.9	58
76	Mn₂FeWO₆: A New Ni₃TeO₆â€Type Polar and Magnetic Oxide. Advanced Materials, 2015, 27, 2177-2181.	11.1	53
77	Adiabatic Pumping of Chern-Simons Axion Coupling. Physical Review Letters, 2015, 114, 096401.	2.9	39
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79	Chern insulator at a magnetic rocksalt interface. Physical Review B, 2014, 90, .	1.1	47
80	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
81	Wannier center sheets in topological insulators. Physical Review B, 2014, 89, .	1.1	139
82	Quantum anomalous Hall phase in (001) double-perovskite monolayers via intersite spin-orbit coupling. Physical Review B, 2014, 90, .	1.1	30
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86	Non-hysteretic colossal magnetoelectricity in a collinear antiferromagnet. Nature Communications, 2014, 5, 3201.	5.8	106
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88	Electrically driven octahedral rotations in SrTiO3and PbTiO3. Physical Review B, 2013, 87, .	1.1	16
89	Chern Insulators from Heavy Atoms on Magnetic Substrates. Physical Review Letters, 2013, 110, 116802.	2.9	99
90	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

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92	Maximally localized Wannier functions: Theory and applications. Reviews of Modern Physics, 2012, 84, 1419-1475.	16.4	2,159
93	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
94	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
95	Spin-phonon coupling effects in transition-metal perovskites: A DFTA+A<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
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97	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
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101	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></mml:math> structure. Physical Review B, 2010, 82, .	1.1	59
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106	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
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110	First-principles theory of magnetically induced ferroelectricity in TbMnO3. European Physical Journal B, 2009, 71, 345-348.	0.6	13
111	A converse approach to the calculation of NMR shielding tensors. Journal of Chemical Physics, 2009, 131, 101101.	1.2	54
112	Magnetoelectric Polarizability and Axion Electrodynamics in Crystalline Insulators. Physical Review Letters, 2009, 102, 146805.	2.9	766
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116	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
117	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
118	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></mml:msub></mml:mrow></mml:math> and (011) surfaces. Physical Review B, 2008, 78, .	1.1	65
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120	Ab initiocalculations 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
121	Suppressed Dependence of Polarization on Epitaxial Strain in Highly Polar Ferroelectrics. Physical Review Letters, 2007, 98, 217602.	2.9	146
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