Vincenzo Fiorentini

List of Publications by Year
in descending order

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149 papers	11,721 citations	46918 47 h-index	27345 106 g-index
152 all docs	152 docs citations	152 times ranked	8342 citing authors

#	Article	IF	Citations
1	Spontaneous polarization and piezoelectric constants of III-V nitrides. Physical Review B, 1997, 56, R10024-R10027.	1.1	2,662
2	Pyroelectric properties of Al(In)GaN/GaN hetero- and quantum well structures. Journal of Physics Condensed Matter, 2002, 14, 3399-3434.	0.7	864
3	Evidence for nonlinear macroscopic polarization in IIIâ€“V nitride alloy heterostructures. Applied Physics Letters, 2002, 80, 1204-1206.	1.5	746
4	Effects of macroscopic polarization in III-V nitride multiple quantum wells. Physical Review B, 1999, 60, 8849-8858.	1.1	488
5	First-principles prediction of structure, energetics, formation enthalpy, elastic constants, polarization, and piezoelectric constants of AlN, GaN, and InN: Comparison of local and gradient-corrected density-functional theory. Physical Review B, 2001, 64, .	1.1	421
6	Macroscopic polarization and band offsets at nitride heterojunctions. Physical Review B, 1998, 57, R9427-R9430.	1.1	371
7	Extracting convergent surface energies from slab calculations. Journal of Physics Condensed Matter, 1996, 8, 6525-6529.	0.7	306
8	Nonlinear macroscopic polarization in III-V nitride alloys. Physical Review B, 2001, 64, .	1.1	272
9	Spontaneous versus Piezoelectric Polarization in III-V Nitrides: Conceptual Aspects and Practical Consequences. Physica Status Solidi (B): Basic Research, 1999, 216, 391-398.	0.7	271
10	Free-carrier screening of polarization fields in wurtzite GaN/InGaN laser structures. Applied Physics Letters, 1999, 74, 2002-2004.	1.5	268
11	Reconstruction mechanism of fcc transition metal (001) surfaces. Physical Review Letters, 1993, 71, 1051-1054.	2.9	262
12	Polarization-Based Calculation of the Dielectric Tensor of Polar Crystals. Physical Review Letters, 1997, 79, 3958-3961.	2.9	236
13	Electronic and structural properties of GaN by the full-potential linear muffin-tin orbitals method: The role of thedelectrons. Physical Review B, 1993, 47, 13353-13362.	1.1	188
14	Spontaneous 2-Dimensional Carrier Confinement at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-Type<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mo>/</mml:mo><mml:msub><mml: Physical Review Letters, 2011, 106, 166807.	2.9	185
15	Accurate calculation of polarization-related quantities in semiconductors. Physical Review B, 2001, 63, .	1.1	168
16	Theoretical Evaluation of Zirconia and Hafnia as Gate Oxides for Si Microelectronics. Physical Review Letters, 2002, 89, 266101.	2.9	167
17	Dielectric scaling of the self-energy scissor operator in semiconductors and insulators. Physical Review B, 1995, 51, 17196-17198.	1.1	142
18	Theory and applications of the stress density. Physical Review B, 2000, 61, 8433-8442.	1.1	139

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19	Theory of adsorption and surfactant effect of Sb on Ag(111). Physical Review Letters, 1993, 71, 2437-2440.	2.9	134
20	First-principles calculation of the piezoelectric tensor dâ‡Š of IIIâ€“V nitrides. Applied Physics Letters, 2002, 80, 4145-4147.	1.5	125
21	Phase diagram and polarization of stable phases of (Ga_{1â^'}) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 662 Td (<sub>	1.1	124
22	Structure and stability of rare-earth and transition-metal oxides. Physical Review B, 2004, 69, .	1.1	114
23	Theoretical evidence for efficient p-type doping of GaN using beryllium. Applied Physics Letters, 1997, 70, 2990-2992.	1.5	102
24	Magnetic Ordering in CuO from First Principles: A Cuprate Antiferromagnet with Fully Three-Dimensional Exchange Interactions. Physical Review Letters, 2005, 95, 086405.	2.9	89
25	Electronic dielectric constants of insulators calculated by the polarization method. Physical Review B, 1998, 58, 15292-15295.	1.1	84
26	Variational pseudo-self-interaction-corrected density functional approach to theab initiodescription of correlated solids and molecules. Physical Review B, 2011, 84, .	1.1	83
27	Local norm-conserving pseudo-Hamiltonians. Physical Review A, 1995, 52, 236-257.	1.0	71
28	Polarization fields in nitride nanostructures: 10 points to think about. Applied Surface Science, 2000, 166, 23-29.	3.1	71
29	Prediction of a native ferroelectric metal. Nature Communications, 2016, 7, 11211.	5.8	71
30	Doping-dependent band structure of LaAlO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>/SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>interfaces by soft x-ray polarization-controlled resonant angle-resolved photoemission. Physical Review B, 2014, 89, .	1.1	70
31	Semiconductor band structures at zero pressure. Physical Review B, 1992, 46, 2086-2091.	1.1	66
32	Exchange interactions and magnetic phases of transition metal oxides: Benchmarking advancedab initiomethods. Physical Review B, 2011, 84, .	1.1	66
33	Electronics and sensors based on pyroelectric AlGaN/GaN heterostructures. Physica Status Solidi C: Current Topics in Solid State Physics, 2003, 0, 1878-1907.	0.8	65
34	Dielectric properties and long-wavelength optical modes of the high-Î°oxideLaAlO3. Physical Review B, 2005, 71, .	1.1	65
35	Coexistence of ionic and metallic bonding in noble-metal oxides. Physical Review B, 2005, 72, .	1.1	64
36	Anomalous relaxations and chemical trends at III-V semiconductor nitride nonpolar surfaces. Physical Review B, 1999, 59, 8026-8031.	1.1	62

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37	Giant oscillating thermopower at oxide interfaces. Nature Communications, 2015, 6, 6678.	5.8	62
38	Theoretical and experimental investigation of optical absorption anisotropy in Î²-Ga₂O₃. Journal of Physics Condensed Matter, 2016, 28, 224005.	0.7	59
39	Theoretical electron affinities of PAHs and electronic absorption spectra of their mono-anions. Astronomy and Astrophysics, 2005, 432, 585-594.	2.1	57
40	Doping screening of polarization fields in nitride heterostructures. Applied Physics Letters, 2000, 76, 3950-3952.	1.5	56
41	Dielectric Properties of High-Î²Oxides: Theory and Experiment forLu2O3. Physical Review Letters, 2005, 94, 027602.	2.9	56
42	Fluorine in Si: Native-defect complexes and the suppression of impurity diffusion. Physical Review B, 2005, 72, .	1.1	53
43	Theoretical evidence for the semi-insulating character of AlN. Journal of Applied Physics, 1999, 85, 2001-2003.	1.1	52
44	The electronic structure of Îµ-Ga2O3. APL Materials, 2019, 7, .	2.2	49
45	Quasiharmonic versus exact surface free energies of Al: A systematic study employing a classical interatomic potential. Physical Review B, 1999, 60, 5055-5064.	1.1	48
46	Structure, energetics, and extrinsic levels of small self-interstitial clusters in silicon. Physical Review B, 2004, 69, .	1.1	48
47	Thermopower in oxide heterostructures: The importance of being multiple-band conductors. Physical Review B, 2012, 86, .	1.1	48
48	Reconstructions of Ir(110) and (100): an ab initio study. Surface Science, 1997, 377-379, 112-116.	0.8	47
49	Proof of the Thermodynamical Stability of theEâ€²Center inSiO2. Physical Review Letters, 2001, 86, 3064-3067.	2.9	46
50	Nonlinear Behavior of Spontaneous and Piezoelectric Polarization in III-V Nitride Alloys. Physica Status Solidi A, 2002, 190, 65-73.	1.7	44
51	A practical first-principles band-theory approach to the study of correlated materials. European Physical Journal B, 2009, 71, 139-183.	0.6	42
52	Ordering and multiple phase transitions in ultrathin nickelate superlattices. Physical Review B, 2012, 86, .	1.1	41
53	Tunable variation of the electron effective mass and exciton radius in hydrogenatedGaAs1âˆ’xNx. Physical Review B, 2004, 69, .	1.1	40
54	Doping-induced dimensional crossover and thermopower burst in Nb-doped SrTiO<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. Physical Review B, 2013, 88, .	1.1	40

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55	Meta-screening and permanence of polar distortion in metallized ferroelectrics. Physical Review B, 2018, 97, .	1.1	39
56	Interplay of strain and magnetism inLa1âˆ'xSrxMnO3from first principles. Physical Review B, 2008, 78, .	1.1	36
57	Ab initio study of oxygen vacancies in Î±-quartz. Journal of Non-Crystalline Solids, 1997, 221, 89-96.	1.5	34
58	Energetics of transient enhanced diffusion of boron in Ge and SiGe. Physical Review B, 2004, 69, .	1.1	34
59	Cation charge anomalies and high-Îºdielectric behavior inDyScO3:Ab initiodensity-functional and self-interaction-corrected calculations. Physical Review B, 2007, 75, .	1.1	34
60	Magnetism of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">La</mml:mi><mml:mn>0.625</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">Sr</mml:mi><mml:mn>0.375</mml:mn></mml:msub><mml:mi mathvariant="normal">Mn</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>under	1.1	31
61	Connection between charge transfer and alloying core-level shifts based on density-functional calculations. Physical Review B, 2000, 61, 5229-5236.	1.1	28
62	Intrinsic origin of two-dimensional electron gas at the (001) surface of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>SrTiO</mml:mtext><mml:mn>3</mml:mn></mml:msub></mml:math>: Physical Review B, 2015, 91, .	1.1	27
63	Origin of the efficient light emission from inversion domain boundaries in GaN. Applied Physics Letters, 2003, 82, 1182-1184.	1.5	26
64	Double-exchange driven ferromagnetic metal-paramagnetic insulator transition in Mn-doped CuO. Physical Review B, 2006, 74, .	1.1	26
65	Semiempirical self-energy corrections to LDA bands of semiconductors, and a scaling law for the scissor operator. Journal of Physics Condensed Matter, 1992, 4, 5967-5976.	0.7	25
66	Jahn-Teller stabilization of magnetic and orbital ordering in rocksalt CuO. Physical Review B, 2009, 80, .	1.1	25
67	Large band offset as driving force of two-dimensional electron confinement: The case of SrTiO<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>/SrZrO<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>interface. Physical Review B, 2013, 88, .	1.1	25
68	Atomistic modeling of large-scale metal film growth fronts. Physical Review B, 1999, 59, R7856-R7859.	1.1	23
69	Viewpoint: Atomic-Scale Design Protocols toward Energy, Electronic, Catalysis, and Sensing Applications. Inorganic Chemistry, 2019, 58, 14939-14980.	1.9	23
70	Ab initio thermal conductivity of thermoelectric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Mg</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>: Evidence for dominant extrinsic effects. Physical Review B, 2018, 98, .	1.1	22
71	Ferromagnetism and Orbital Order in a Topological Ferroelectric. Physical Review Letters, 2012, 109, 217202.	2.9	21
72	Hydrogen, Acceptors, and H-Acceptor Complexes in GaN. Materials Research Society Symposia Proceedings, 1995, 395, 503.	0.1	20

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73	Towards an understanding of surfactant action in the epitaxial growth of metals: The case of Sb on Ag (111). Applied Physics A: Materials Science and Processing, 1995, 60, 399-402.	1.1	19
74	Bound states of the Fe impurity in wurtzite GaN from hybrid density-functional calculations. Physical Review B, 2011, 84, .	1.1	19
75	Low In solubility and band offsets in the small-xÎ²-Ga₂O₃/(Ga_{1âˆ’}_xIn_x₂<sub>O< Applied Physics Express, 2015, 8, 021102.	1.1	19
76	Extracting convergent surface formation energies from slab calculations. Journal of Physics Condensed Matter, 1998, 10, 895-895.	0.7	18
77	Anomalous energetics and defect-assisted diffusion of Ga in silicon. Applied Physics Letters, 2004, 85, 4902-4904.	1.5	18
78	First-principles calculation of electronic and structural properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>YBa</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms Physical Review B, 2010, 82, .	1.1	17
79	Stability of Ge-related point defects and complexes in Ge-dopedSiO2. Physical Review B, 2002, 66, .	1.1	16
80	Dielectric properties of two phases of crystalline lutetium oxide. Microelectronics Reliability, 2005, 45, 831-833.	0.9	16
81	Magnetic Ordering under Strain and Spin-Peierls Dimerization inGeCuO3. Physical Review Letters, 2007, 98, 196403.	2.9	16
82	Dielectric constant boost in amorphous sesquioxides. Applied Physics Letters, 2008, 92, .	1.5	16
83	Efficient thermoelectricity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sr</mml:mi><mml:mn>2</mml:mn></mml:mrow><mml:mrow><mml:mi mathvariant="normal">O</mml:mi><mml:mn>7</mml:mn></mml:msub></mml:mrow></mml:math> with energy-dependent relaxation times. Physical Review Materials, 2020, 4, .	0.9	16
84	Faceting and stress of missing-row reconstructed transition-metal (110) surfaces. Physical Review B, 1999, 60, 14366-14371.	1.1	15
85	Theory of thermoelectricity in Mg₃Sb₂ with an energy- and temperature-dependent relaxation time. Journal of Physics Condensed Matter, 2019, 31, 065702.	0.7	15
86	Band offsets and stability of BeTe/ZnSe (100) heterojunctions. Physical Review B, 2000, 62, R16302-R16305.	1.1	14
87	Large fluorine-vacancy clusters in Si and their capture efficiency for self-interstitials. Applied Physics Letters, 2006, 89, 092113.	1.5	14
88	Multiferroicity and orbital ordering in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Pr</mml:mtext></mml:mrow><mml:mrow><mml:mn>1 first principles. Physical Review B, 2010, 82, .	1.1	14
89	Multiscale approaches for metal thin film growth. Computational Materials Science, 2002, 24, 58-65.	1.4	13
90	Te-induced modulation of the Moâ€¢HfO2 interface effective work function. Applied Physics Letters, 2008, 92, .	1.5	13

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91	Chain metallicity and competition between paramagnetism and antiferromagnetism in underdoped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>YBa</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>A first principles de. Physical Review B, 2008, 78, .	1.1	13
92	Multiferroicity in vanadium-doped La2Ti2O7: insights from first principles. European Physical Journal B, 2013, 86, 1.	0.6	12
93	Lattice constant, effective mass, and gap recovery in hydrogenatedGaAs1âˆ’xNx. Physical Review B, 2004, 69, .	1.1	11
94	Comparison between experimental and theoretical determination of the local structure of theGaAs1âˆ’yNydilute nitride alloy. Physical Review B, 2005, 71, .	1.1	11
95	Fermi-surface pockets in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>YBa</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>Comparison ofab initiotechniques. Physical Review B, 2009, 79, .	1.1	11
96	Band alignment at Cu2O/La0.7Sr0.3MnO3 interface: A combined experimental-theoretical determination. Applied Physics Letters, 2010, 97, .	1.5	11
97	Reorientable dipolar<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mrow><mml:mtext>Ca</mml:mtext></mml:mrow></mml:math>and anomalous screening in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CaCu</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>Physical Review B, 2010, 81, .	1.1	11
98	Surface antiferromagnetism and incipient metal-insulator transition in strained manganite films. Physical Review B, 2013, 87, .	1.1	11
99	High thermoelectric figure of merit and thermopower in layered perovskite oxides. Physical Review Materials, 2019, 3, .	0.9	11
100	Effective-mass single and double acceptor spectra in GaAs. Physical Review B, 1995, 51, 10161-10163.	1.1	10
101	Complexes, clustering, and native-defect-assisted diffusion of aluminum in silicon. Physical Review B, 2004, 70, .	1.1	10
102	Conservation of dielectric constant upon amorphization in perovskite oxides. Physical Review B, 2007, 76, .	1.1	10
103	Magnetism and unusual Cu valency in quadruple perovskites. European Physical Journal B, 2012, 85, 1.	0.6	10
104	Properties of (Ga_{1âˆ’x}In_x)₂O₃ over the whole x range. Journal of Physics Condensed Matter, 2016, 28, 224001.	0.7	10
105	Interpretation of double acceptor spectra in Ge. Solid State Communications, 1989, 69, 953-958.	0.9	9
106	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
107	Metal-insulator transitions and singlet polarons in one-dimensional<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ca</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:math>Physical Review B, 2008, 77, .	1.1	9
108	Structure and gap of low-x(Ga_{1-x}In_x)₂O₃alloys. Journal of Physics: Conference Series, 2014, 566, 012016.	0.3	9

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109	Impurity-vacancy complexes and ferromagnetism in doped sesquioxides. Physical Review B, 2014, 89, .	1.1	9
110	Offsets and Polarization at Strained AlN/GaN Polar Interfaces. Materials Research Society Symposia Proceedings, 1996, 449, 923.	0.1	8
111	Inhibited Al Diffusion and Growth Roughening of Ga-Coated Al(100). Physical Review Letters, 1996, 77, 695-698.	2.9	8
112	Ionicity and Relaxation Anomalies at IIIâ€“V Nitride Surfaces. Physica Status Solidi A, 1998, 170, 265-269.	1.7	8
113	No In-Plane Reconstruction of Cu(001). Physical Review Letters, 1998, 81, 4278-4278.	2.9	8
114	Incorporation, diffusion, and electrical activity of Li in GaN. Physical Review B, 2000, 61, 12598-12601.	1.1	8
115	Comment on â€œAbÂInitioCalculations to Model Anomalous Fluorine Behaviorâ€. Physical Review Letters, 2006, 96, 039601; discussion 039602.	2.9	8
116	Dielectric and vibrational properties of bixbyite sesquioxides. Physical Review B, 2009, 80, .	1.1	8
117	A three-order-parameter bistable magnetoelectric multiferroic metal. Nature Communications, 2020, 11, 4922.	5.8	8
118	Vibrational modes of three-membered self-interstitial clusters in silicon. Journal of Physics Condensed Matter, 2003, 15, 7851-7857.	0.7	7
119	Structure and Quasiparticle Energies of Cubic, Wurtzite and Hexagonal BN. Materials Research Society Symposia Proceedings, 1995, 395, 429.	0.1	6
120	Influence of point defects injection on the stability of a supersaturatedGaâ€Sisolid solution. Physical Review B, 2005, 71, .	1.1	6
121	Multiferroicity in V-doped PbTiO₃. Journal of Physics: Conference Series, 2013, 470, 012013.	0.3	6
122	Electronic Structure of Bulk and Defected CaCu3Ti4O12. ECS Transactions, 2006, 3, 291-297.	0.3	5
123	Self-interaction-free density-functional band theory for magnetic cuprates. Journal of Magnetism and Magnetic Materials, 2007, 310, 1648-1650.	1.0	5
124	Formation Energy, Stress, and Relaxations of Low-Index Rhodium Surfaces. Materials Research Society Symposia Proceedings, 1995, 408, 457.	0.1	4
125	Roughening of close-packed singular surfaces. Physical Review B, 2001, 63, .	1.1	4
126	Magnetic couplings vs. stress and strain in epitaxial (La, Sr)MnO3. European Physical Journal B, 2009, 70, 343-346.	0.6	4

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127	Topological multiferroics. Phase Transitions, 2015, 88, 953-961.	0.6	4
128	Self-consistent DFT calculations of electronic states in superlattices and quantum wells with arbitrary compositional and doping profiles. Semiconductor Science and Technology, 1990, 5, 211-217.	1.0	3
129	Stress and reconstruction on (001) transition-metal surfaces. Computational Materials Science, 2001, 20, 423-428.	1.4	3
130	Ordered versus disordered growth of copper quantum wires on Mo and W vicinal surfaces. Physical Review B, 2003, 67, .	1.1	3
131	Modeling of Alternative High-k Dielectrics for Memory Based Applications. ECS Transactions, 2009, 25, 131-145.	0.3	3
132	Giant electroresistance and tunable magnetoelectricity in a multiferroic junction. Physical Review B, 2013, 88, .	1.1	3
133	Vibrational stability of graphene under combined shear and axial strains. Physical Review B, 2015, 92, .	1.1	3
134	Influence of thermal conductivity and of non-constant relaxation time on thermoelectricity in Mg₃Sb₂. Journal of Physics: Conference Series, 2019, 1226, 012010.	0.3	3
135	Giant thermoelectric figure of merit in multivalley high-complexity-factor LaSO. Physical Review Materials, 2021, 5, .	0.9	3
136	A note on AB INITIO semiconductor band structures. Solid State Communications, 1992, 83, 871-875.	0.9	2
137	Dielectric Properties of Rare-Earth Oxides: General Trends from Theory. , 0, , 225-246.		2
138	Indium on Cu(100) from first principles: Energetics, complex formation, and diffusion of adsorbates and vacancies on terraces and at steps. Physical Review B, 2009, 79, .	1.1	2
139	Fermi-surface pockets in magnetic underdoped cuprates from first principles. Europhysics Letters, 2009, 88, 67009.	0.7	2
140	Multigap absorption inCaCu3Ti4O12and the prediction capability ofab initiomethods. Physical Review B, 2014, 90, .	1.1	2
141	Surface Alloying and Surfactant Action of Sb ON Ag (111). Materials Research Society Symposia Proceedings, 1993, 317, 323.	0.1	1
142	Tuning of the electron effective mass and exciton wavefunction size in GaAs1â^'xNx. Physica E: Low-Dimensional Systems and Nanostructures, 2004, 21, 747-751.	1.3	1
143	Publisher's Note: Dielectric and vibrational properties of bixbyite sesquioxides [Phys. Rev. B80, 104301 (2009)]. Physical Review B, 2009, 80, .	1.1	1
144	Singling out the effect of quenched disorder in the phase diagram of cuprates. Journal of Physics Condensed Matter, 2019, 31, 184002.	0.7	1

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145	A Theoretical View on the Dielectric Properties of Crystalline and Amorphous High-Îº Materials and Films. , 2007, , 269-292.		1
146	Simulated Thermal Effects on Structural and Electronic Properties of GaN. Materials Research Society Symposia Proceedings, 1995, 395, 435.	0.1	0
147	Electronic properties and doping mechanism in cuprates by first-principles calculations. , 2008, , .		0
148	Publisher's Note: Dielectric and vibrational properties of bixbyite sesquioxides [Phys. Rev. B80, 104301 (2009)]. Physical Review B, 2009, 80, .	1.1	0
149	Homoepitaxial Growth of Metals and the Role of Surfactants. , 1996, , 219-231.		0