Peter Blaha

List of Publications by Year in descending order

354 papers	33,545 citations	8159 76 h-index	4203 174 g-index
367 all docs	367 docs citations	367 times ranked	22381 citing authors

#	Article	IF	Citations
1	Accurate Band Gaps of Semiconductors and Insulators with a Semilocal Exchange-Correlation Potential. Physical Review Letters, 2009, 102, 226401.	2.9	4,279
2	Full-potential, linearized augmented plane wave programs for crystalline systems. Computer Physics Communications, 1990, 59, 399-415.	3.0	3,005
3	Electronic structure calculations of solids using the WIEN2k package for material sciences. Computer Physics Communications, 2002, 147, 71-76.	3.0	1,582
4	WIEN2k: An APW+lo program for calculating the properties of solids. Journal of Chemical Physics, 2020, 152, 074101.	1.2	1,185
5	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
6	Solid state calculations using WIEN2k. Computational Materials Science, 2003, 28, 259-273.	1.4	1,008
7	Efficient linearization of the augmented plane-wave method. Physical Review B, 2001, 64, .	1.1	914
8	Merits and limits of the modified Becke-Johnson exchange potential. Physical Review B, 2011, 83, .	1.1	743
9	Accurate Density Functional with Correct Formal Properties: A Step Beyond the Generalized Gradient Approximation. Physical Review Letters, 1999, 82, 2544-2547.	2.9	731
10	Calculation of the lattice constant of solids with semilocal functionals. Physical Review B, 2009, 79, .	1.1	709
11	Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs. , 1999, 75, 889-909.		598
12	Improving the modified Becke-Johnson exchange potential. Physical Review B, 2012, 85, .	1.1	552
13	Lattice dynamics and hyperfine interactions in ZnO and ZnSe at high external pressures. Physical Review B, 1996, 53, 11425-11438.	1.1	509
14	Applications of Engel and Voskoâ€™s generalized gradient approximation in solids. Physical Review B, 1994, 50, 7279-7283.	1.1	359
15	Hybrid exchange-correlation energy functionals for strongly correlated electrons: Applications to transition-metal monoxides. Physical Review B, 2006, 74, .	1.1	309
16	Performance on molecules, surfaces, and solids of the Wu-Cohen GGA exchange-correlation energy functional. Physical Review B, 2007, 75, .	1.1	306
17	First-Principles Calculation of the Electric Field Gradient ofLi3N. Physical Review Letters, 1985, 54, 1192-1195.	2.9	289
18	First-principles calculation of the electric-field gradient in hcp metals. Physical Review B, 1988, 37, 2792-2796.	1.1	284

#	Article	IF	Citations
19	Towards efficient band structure and effective mass calculations for III-V direct band-gap semiconductors. Physical Review B, 2010, 82, .	1.1	279
20	Improving the efficiency of FP-LAPW calculations. Computer Physics Communications, 2000, 126, 294-309.	3.0	252
21	Determination of the Nuclear Quadrupole Moment of57Fe. Physical Review Letters, 1995, 75, 3545-3548.	2.9	251
22	Electronic structure and transport in type-I and type-VIII clathrates containing strontium, barium, and europium. Physical Review B, 2003, 68, .	1.1	251
23	Carbon monoxide-induced adatom sintering in a Pdâ€“Fe3O4 model catalyst. Nature Materials, 2013, 12, 724-728.	13.3	249
24	Charge distribution and electric-field gradients inYBa2Cu3O7â^'x. Physical Review B, 1990, 42, 2051-2061.	1.1	248
25	Spin-orbit splitting of theL-gap surface state on Au(111) and Ag(111). Physical Review B, 2001, 65, .	1.1	243
26	Subsurface cation vacancy stabilization of the magnetite (001) surface. Science, 2014, 346, 1215-1218.	6.0	222
27	Electronic structure of fcc Th: Spin-orbit calculation with6p1/2local orbital extension. Physical Review B, 2001, 64, .	1.1	219
28	Boron Nitride Nanomesh: Functionality from a Corrugated Monolayer. Angewandte Chemie - International Edition, 2007, 46, 5115-5119.	7.2	209
29	Band gap calculations with Beckeâ€“Johnson exchange potential. Journal of Physics Condensed Matter, 2007, 19, 196208.	0.7	195
30	Rungs 1 to 4 of DFT Jacobâ€™s ladder: Extensive test on the lattice constant, bulk modulus, and cohesive energy of solids. Journal of Chemical Physics, 2016, 144, 204120.	1.2	191
31	Electric-field-gradient calculations using the projector augmented wave method. Physical Review B, 1998, 57, 14690-14697.	1.1	187
32	Density functional theory investigation of the geometric and spintronic structure ofh-BN/Ni(111) in view of photoemission and STM experiments. Physical Review B, 2003, 68, .	1.1	179
33	Surface Trapping of Atoms and Molecules with Dipole Rings. Science, 2008, 319, 1824-1826.	6.0	163
34	Electronic and magnetic structure of BCC Fe-Co alloys from band theory. Journal of Physics F: Metal Physics, 1984, 14, 2659-2671.	1.6	159
35	Implementation of screened hybrid functionals based on the Yukawa potential within the LAPW basis set. Physical Review B, 2011, 83, .	1.1	159
36	Spectroscopic Signatures of Spin-Charge Separation in the Quasi-One-Dimensional Organic Conductor TTF-TCNQ. Physical Review Letters, 2002, 88, 096402.	2.9	157

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37	Bonding of hexagonal BN to transition metal surfaces: Anab initiodensity-functional theory study. Physical Review B, 2008, 78, .	1.1	156
38	Magnetic structure and electric-field gradients of uranium dioxide: Anab initiostudy. Physical Review B, 2004, 69, .	1.1	155
39	Electronic structure of 3d-transition-metal oxides: on-site Coulomb repulsion versus covalency. Journal of Physics Condensed Matter, 1999, 11, 1657-1682.	0.7	151
40	Single-Layer Model of the Hexagonal Boron Nitride Nanomesh on the Rh(111) Surface. Physical Review Letters, 2007, 98, 106802.	2.9	147
41	Three-Dimensional Electron Realm in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>VSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>by Soft-X-Ray Photoelectron Spectroscopy: Origin of Charge-Density Waves. Physical Review Letters, 2012, 109, 086401.	2.9	144
42	Spin-State Crossover and Hyperfine Interactions of Ferric Iron in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>MgSiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Perovskite. Physical Review Letters, 2011, 106, 118501.	2.9	143
43	Electron densities and chemical bonding in TiC, TiN, and TiO derived from energy band calculations. International Journal of Quantum Chemistry, 1983, 23, 1535-1552.	1.0	134
44	Electronic structure of solids with WIEN2k. Molecular Physics, 2010, 108, 3147-3166.	0.8	133
45	Generalized-gradient-approximation description of band splittings in transition-metal oxides and fluorides. Physical Review B, 1994, 49, 10170-10175.	1.1	130
46	Importance of the Kinetic Energy Density for Band Gap Calculations in Solids with Density Functional Theory. Journal of Physical Chemistry A, 2017, 121, 3318-3325.	1.1	126
47	Understanding the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>L</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mo>,</mml:mo><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>absorption spectra of early<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>transition elements. Physical Review B, 2010, 82, .	1.1	125
48	The theoretical charge density of silicon: experimental testing of exchange and correlation potentials. Journal of Physics Condensed Matter, 1997, 9, 7541-7561.	0.7	124
49	Theory of orientation-sensitive near-edge fine-structure core-level spectroscopy. Physical Review B, 1999, 59, 12807-12814.	1.1	120
50	Charge-Density-Wave Mechanism in2Hâ^'NbSe2: Photoemission Results. Physical Review Letters, 1999, 82, 4504-4507.	2.9	117
51	Ab initiostudy of the martensitic bcc-hcp transformation in iron. Physical Review B, 1998, 58, 5296-5304.	1.1	115
52	Oxide Heterostructures for Efficient Solar Cells. Physical Review Letters, 2013, 110, 078701.	2.9	113
53	Electric-field-gradient calculations for systems with large extended-core-state contributions. Physical Review B, 1992, 46, 1321-1325.	1.1	108
54	Itinerant metamagnetism and possible spin transition in LaCoO[sub 3] by temperature/hole doping. Journal of Applied Physics, 2002, 91, 291.	1.1	108

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55	DFT Study of the Role of Al³⁺ in the Fast Ion-Conductor Li_{7â€“3x}Al³⁺_xLa₃Zr₂O₁₂ Garnet. Chemistry of Materials, 2014, 26, 2617-2623.	9.2	108
56	Dual role of CO in the stability of subnano Pt clusters at the Fe ₃ O ₄ (001) surface. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 8921-8926.	3.3	108
57	Electronic structure of the quasi-one-dimensional organic conductor TTF-TCNQ. Physical Review B, 2003, 68, .	1.1	106
58	Electronic structure of the mixed valence system(YM)2BaNiO5â€,(M=Ca,Sr). Physical Review B, 2001, 63, .	1.1	104
59	Competing structural instabilities in the ferroelectric Aurivillius compoundSrBi2Ta2O9. Physical Review B, 2004, 70, .	1.1	104
60	Spin states and hyperfine interactions of iron in (Mg,Fe)SiO3 perovskite under pressure. Earth and Planetary Science Letters, 2010, 294, 19-26.	1.8	102
61	Magnetic order and defect structure ofFexAl1â^'xalloys aroundx=0.5:â€ƒAn experimental and theoretical study. Physical Review B, 1998, 58, 14922-14933.	1.1	100
62	Metallic â€œFerroelectricityâ€•in the PyrochloreCd2Re2O7. Physical Review Letters, 2004, 92, 065501.	2.9	100
63	Charge distribution and chemical bonding inCu2O. Physical Review B, 2003, 67, .	1.1	98
64	Electronic structure of hcp metals. Physical Review B, 1988, 38, 9368-9374.	1.1	96
65	Correlation Induced Paramagnetic Ground State in FeAl. Physical Review Letters, 2001, 87, 196401.	2.9	95
66	Electronic Structure and Optical Properties of AFeO2(A = Ag, Cu) within GGA Calculations. Chemistry of Materials, 2007, 19, 634-640.	3.2	95
67	Bonding study of TiC and TiN. II. Theory. Physical Review B, 1985, 31, 2316-2325.	1.1	94
68	Comment on â€œTaming multiple valency with density functionals: A case study of defective ceriaâ€• Physical Review B, 2005, 72, .	1.1	90
69	Atomic-Scale Structure of the Hematite Î±-Fe₂O₃(11Ì…02) â€œR-Cutâ€•Surface. Journal of Physical Chemistry C, 2018, 122, 1657-1669.	1.5	89
70	Mo cluster formation in the intercalation compoundLiMoS2. Physical Review B, 2000, 62, 2397-2400.	1.1	87
71	Occupied and unoccupied electronic band structure ofWSe2. Physical Review B, 1997, 55, 10400-10411.	1.1	84
72	Construction of an optimal GGA functional for molecules and solids. Physical Review B, 2011, 83, .	1.1	84

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73	Electronic structure and binding mechanism of Cu2O. European Physical Journal B, 1986, 64, 119-127.	0.6	82
74	Electronic structure of the pyrochlore metalsCd2Os2O7andCd2Re2O7. Physical Review B, 2002, 65, .	1.1	81
75	Magnetic and half-metallic properties of the full-Heusler alloys Co2TiX(X=Al,Ga;Si,Ge,Sn;Sb). Journal of Applied Physics, 2005, 97, 10C307.	1.1	81
76	Electronic Quasiparticle Renormalization on the Spin Wave Energy Scale. Physical Review Letters, 2004, 92, 097205.	2.9	80
77	Pressure-induced phase transitions in solid Si,SiO2,and Fe: Performance of local-spin-density and generalized-gradient-approximation density functionals. Physical Review B, 1998, 58, 11266-11272.	1.1	77
78	Strong excitonic effects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CuAlO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> transparent conductive oxides. Physical Review B, 2009, 79, .	1.1	76
79	Room-temperature spin-spiral multiferroicity in high-pressure cupric oxide. Nature Communications, 2013, 4, 2511.	5.8	76
80	Adsorption and incorporation of transition metals at the magnetite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>(001) surface. Physical Review B, 2015, 92, .	1.1	76
81	Epitaxial growth of hexagonal boron nitride on Ag(111). Physical Review B, 2010, 82, .	1.1	75
82	Electronic Structure Study of CO Adsorption on the Fe(001) Surface. Journal of Physical Chemistry B, 2001, 105, 164-172.	1.2	74
83	Temperature and composition dependence of crystal structures and magnetic and electronic properties of the double perovskites<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>La</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn> Physical Review B, 2010, 82, .	1.1	74
84	Hybrid functionals for solids with an optimized Hartreeâ€“Fock mixing parameter. Journal of Physics Condensed Matter, 2013, 25, 435503.	0.7	74
85	Calculations of electric field gradients in solids: How theory can complement experiment. , 2000, 126, 389-395.		72
86	Rare earth borocarbides: Electronic structure calculations and electric field gradients. Physical Review B, 2000, 62, 6774-6785.	1.1	72
87	Insight into the performance of GGA functionals for solid-state calculations. Physical Review B, 2009, 80, .	1.1	72
88	Assessment of DFT functionals with NMR chemical shifts. Physical Review B, 2013, 87, .	1.1	72
89	The orientation-dependent simulation of ELNES. Ultramicroscopy, 2000, 83, 9-16.	0.8	70
90	The fcc - bcc structural transition: I. A band theoretical study for Li, K, Rb, Ca, Sr, and the transition metals Ti and V. Journal of Physics Condensed Matter, 1996, 8, 799-815.	0.7	69

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91	Absolute Band Mapping by Combined Angle-Dependent Very-Low-Energy Electron Diffraction and Photoemission: Application to Cu. Physical Review Letters, 1998, 81, 4943-4946.	2.9	69
92	Electronic structure and electric-field gradients forYBa2Cu4O8from density-functional calculations. Physical Review B, 1991, 44, 5141-5147.	1.1	68
93	Electron-density distribution in stishovite, SiO2: aÂnew high-energy synchrotron-radiation study. Acta Crystallographica Section A: Foundations and Advances, 2001, 57, 663-677.	0.3	68
94	Three-dimensional unoccupied band structure of graphite: Very-low-energy electron diffraction and band calculations. Physical Review B, 2000, 61, 4994-5001.	1.1	66
95	Ferromagnetic insulating state in tensile-strained LaCoO<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>thin films from LDA<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo>+</mml:mo></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>U</mml:mi></mml:math>	1.1	66
96	Fermi surface and electron correlation effects of ferromagnetic iron. Physical Review B, 2005, 72, .	1.1	65
97	Nonlocal van der Waals functionals for solids: Choosing an appropriate one. Physical Review Materials, 2019, 3, .	0.9	65
98	Electron density distribution and bond critical point properties for forsterite, Mg2 SiO4, determined with synchrotron single crystal X-ray diffraction data. Physics and Chemistry of Minerals, 2005, 32, 301-313.	0.3	64
99	Origin of the light green color and electronic ground state ofLaCrO3. Physical Review B, 2008, 77, .	1.1	63
100	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m linearized augmented plane waves extended by high-energy local orbitals. Physical Review B, 2016, 93, .	1.1	63
101	A full-potential LAPW study of structural and electronic properties of beryllium. Journal of Physics F: Metal Physics, 1987, 17, 899-911.	1.6	62
102	High-Temperature Symmetry Breaking in the Electronic Band Structure of the Quasi-One-Dimensional SolidNbSe3. Physical Review Letters, 2001, 87, 196403.	2.9	62
103	Ab initiostudy of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>h</mml:mi><mml:mtext>â^'</mml:mtext><mml:mtext>BN</mml:mtext></mml:math>nanomeshes on Ru(001), Rh(111), and Pt(111). Physical Review B, 2010, 81, .	1.1	61
104	Electronically Driven Soft Modes in Zinc Metal. Physical Review Letters, 1995, 74, 1139-1142.	2.9	60
105	Electronic structure and chemical bonding effects upon the bcc toÎ©phase transition:Ab initiostudy of Y, Zr, Nb, and Mo. Physical Review B, 2000, 62, 12743-12753.	1.1	60
106	Theoretical Investigation of the Magnetic Exchange Interactions in Copper(II) Oxides under Chemical and Physical Pressures. Scientific Reports, 2012, 2, 759.	1.6	59
107	Structure and properties of CoMnSb in the context of half-metallic ferromagnetism. Physical Review B, 2006, 74, .	1.1	58
108	Optical properties and band structure of2Hâ^'WSe2. Physical Review B, 1999, 60, 8610-8615.	1.1	57

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109	Multiple instabilities in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Bi</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">Ti</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>12</mml:mn></mml:msub></mml:mrow></mml:math>: A ferroelectric beyond the soft-mode paradigm. Physical Review B, 2008, 77, .	1.1	53
110	Giant spontaneous Hall effect in a nonmagnetic Weylâ€“Kondo semimetal. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	53
111	Calculation of electric hyperfine interaction parameters in solids. Hyperfine Interactions, 1996, 97-98, 1-10.	0.2	51
112	Partial core hole screening in the Cu L 3 edge. European Physical Journal B, 2001, 21, 363-367.	0.6	51
113	Cluster Nucleation and Growth from a Highly Supersaturated Adatom Phase: Silver on Magnetite. ACS Nano, 2014, 8, 7531-7537.	7.3	51
114	Direct Spectroscopic Observation of the Energy Gap Formation in the Spin Density Wave Phase Transition at the Cr(110) Surface. Physical Review Letters, 1999, 83, 2069-2072.	2.9	49
115	Group V acceptors in CdTe:Ab initiocalculation of lattice relaxation and the electric-field gradient. Physical Review B, 2000, 62, R2259-R2262.	1.1	49
116	Magnetism in the Huesler alloys: Co2TiSn and Co2TiAl. Journal of Magnetism and Magnetic Materials, 1995, 140-144, 183-184.	1.0	48
117	Recovering experimental and theoretical electron densities in corundum using the multipolar model: IUCr Multipole Refinement Project. Acta Crystallographica Section A: Foundations and Advances, 2001, 57, 290-303.	0.3	46
118	Ordered Mesoporous TiO₂ Gyroids: Effects of Pore Architecture and Nbâ€Doping on Photocatalytic Hydrogen Evolution under UV and Visible Irradiation. Advanced Energy Materials, 2018, 8, 1802566.	10.2	46
119	Ab initio calculation of electric-field-gradient tensors of forsterite. American Mineralogist, 1996, 81, 545-549.	0.9	46
120	Cobalt spin states and hyperfine interactions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaCoO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>by<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>LDA</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math>: Physical Review B, 2010, 82, .	1.1	44
121	Assessment of the GLLB-SC potential for solid-state properties and attempts for improvement. Physical Review Materials, 2018, 2, .	0.9	44
122	Structure and stability ofCd2Nb2O7andCd2Ta2O7explored byab initiocalculations. Physical Review B, 2008, 78, .	1.1	43
123	Accounting for spin fluctuations beyond local spin density approximation in the density functional theory. Physical Review B, 2012, 86, .	1.1	43
124	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>F</mml:mi></mml:math>center in lithium fluoride revisited: Comparison of solid-state physics and quantum-chemistry approaches. Physical Review B, 2014, 89, .	1.1	43
125	Electronic structure and heavy-fermion behavior inLiV2O4. Physical Review B, 1999, 60, 16359-16363.	1.1	42
126	Three-dimensional band mapping by angle-dependent very-low-energy electron diffraction and photoemission: Methodology and application to Cu. Physical Review B, 2001, 63, .	1.1	42

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127	Electronic structure of CrN: A comparison between different exchange correlation potentials. Physical Review B, 2012, 85, .	1.1	42
128	Electronic structure and electric field gradient calculations of Al 2 SiO 5 polymorphs. Physics and Chemistry of Minerals, 2001, 28, 67-75.	0.3	41
129	Unraveling the structure of the h-BN/Rh(111) nanomesh withab initiocalculations. Journal of Physics Condensed Matter, 2008, 20, 064207.	0.7	41
130	Calculations of NMR chemical shifts with APW-based methods. Physical Review B, 2012, 85, .	1.1	41
131	Magnetocrystalline anisotropy of FePt: A detailed view. Physical Review B, 2016, 94, .	1.1	41
132	Semilocal exchange-correlation potentials for solid-state calculations: Current status and future directions. Journal of Applied Physics, 2019, 126, .	1.1	41
133	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow><mml:mn>2</mml:mn><mml:mi>g</mml:mi></mml:mrow></mml:msub> dispersion and spin polarization in thin films of Fe<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>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow />	1.1	40
134	On the existence of non-nuclear maxima in simple metals. Journal of Chemical Physics, 2002, 117, 8030-8035.	1.2	39
135	Calculating NMR chemical shifts using the augmented plane-wave method. Physical Review B, 2014, 89, .	1.1	39
136	Electronic structure of1Tâ^'TiS2. Physical Review B, 1999, 59, 14833-14836.	1.1	38
137	Fermi Surface of Three-Dimensional<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>La</mml:mi></mml:mrow><mml:mrow><mml:mn>1</mml:mn> by Soft-X-Ray ARPES: Rhombohedral Lattice Distortion and its Effect. Physical Review Letters, 2015, 114, 237601.	2.9	38
138	Investigation of the Optical and Excitonic Properties of the Visible Light-Driven Photocatalytic BiVO₄ Material. Chemistry of Materials, 2017, 29, 3380-3386.	3.2	38
139	Systematic investigation of a family of gradient-dependent functionals for solids. Physical Review B, 2010, 81, .	1.1	36
140	Band Gap Extraction from Individual Two-Dimensional Perovskite Nanosheets Using Valence Electron Energy Loss Spectroscopy. Journal of Physical Chemistry C, 2016, 120, 11170-11179.	1.5	36
141	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>PBE</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math>calcu of the Jahn-Teller effect in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Pr</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2008, 77, .	1.1	35
142	Influence of reconstruction on the surface state of Au(110). Physical Review B, 2008, 78, .	1.1	35
143	Density functional calculations on the charge-ordered and valence-mixed modification of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>YBaFe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml: Physical Review B, 2009, 79, .	1.1	35
144	Short-range magnetic order and temperature-dependent properties of cupric oxide. Journal of Physics Condensed Matter, 2010, 22, 045502.	0.7	35

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145	Electronic and magnetic structure ofMnF2andNiF2. Physical Review B, 1993, 48, 12672-12681.	1.1	34
146	Ab initio Calculations of the Electric Field Gradients in Solids in Relation to the Charge Distribution. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1992, 47, 197-202.	0.7	33
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