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	WloopPHI: A tool for ab initio characterization of Weyl semimetals. Computer Physics Communications, 2022, 270, 108147.	3.0	5
2	Length-Gauge Optical Matrix Elements in WIEN2k. Computation, 2022, 10, 22.	1.0	2
3	CO Adsorption and Disproportionation on Smooth and Defect-Rich Ir(111). Journal of Physical Chemistry C, 2022, 126, 6578-6589.	1.5	3
4	Dedication: Commemorative Issue in Honor of Professor Karlheinz Schwarz on the Occasion of His 80th Birthday. Computation, 2022, 10, 78.	1.0	0
5	Implementation of self-consistent MGGA functionals in augmented plane wave based methods. Physical Review B, 2022, 105, .	1.1	4
6	What is the optimal mGGA exchange functional for solids?. Journal of Chemical Physics, 2022, 157, .	1.2	3
7	Perturbation approach to ab initio effective mass calculations. Computer Physics Communications, 2021, 261, 107648.	3.0	21
8	Elucidating the formation and active state of Cu co-catalysts for photocatalytic hydrogen evolution. Journal of Materials Chemistry A, 2021, 9, 21958-21971.	5.2	17
9	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
10	Light emission from direct band gap germanium containing split-interstitial defects. Physical Review B, 2021, 103, .	1.1	11
11	First-principles self-consistent phonon approach to the study of the vibrational properties and structural phase transition of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><m Physical Review B, 2021, 103, .	1.1	11
12	Efficient Band Structure Calculation of Two-Dimensional Materials from Semilocal Density Functionals. Journal of Physical Chemistry C, 2021, 125, 11206-11215.	1.5	19
13	Pristine quantum criticality in a Kondo semimetal. Science Advances, 2021, 7, .	4.7	11
14	Bandgap of two-dimensional materials: Thorough assessment of modern exchangeâ€“correlation functionals. Journal of Chemical Physics, 2021, 155, 104103.	1.2	26
15	125Te NMR for structural investigations in phase change materials: Optimization of experimental conditions coupled to NMR shift prediction. Solid State Nuclear Magnetic Resonance, 2021, 115, 101751.	1.5	1
16	Density analysis for estimating the degree of on-site correlation on transition-metal atoms in extended systems. Physical Review B, 2021, 104, .	1.1	0
17	Density Functional Theory Study of Metal and Metal-Oxide Nucleation and Growth on the Anatase TiO2(101) Surface. Computation, 2021, 9, 125.	1.0	2
18	Stress tensor in the linearized augmented plane wave method. Physical Review B, 2021, 104, .	1.1	2

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19	Measurement of electric quadrupole moment in neutron rich ^{131,132}I. European Physical Journal A, 2020, 56, 1.	1.0	0
20	Shortcomings of meta-GGA functionals when describing magnetism. Physical Review B, 2020, 102, .	1.1	27
21	Coverage-Induced Orientation Change: CO on Ir(111) Monitored by Polarization-Dependent Sum Frequency Generation Spectroscopy and Density Functional Theory. Journal of Physical Chemistry C, 2020, 124, 18102-18111.	1.5	9
22	Modifying the Surface Structure of Perovskite-Based Catalysts by Nanoparticle Exsolution. Catalysts, 2020, 10, 268.	1.6	32
23	Local geometry around B atoms in B/Si(1â€‰1â€‰1) from polarized x-ray absorption spectroscopy. Journal of Physics Condensed Matter, 2020, 32, 045901.	0.7	1
24	WIEN2k: An APW+lo program for calculating the properties of solids. Journal of Chemical Physics, 2020, 152, 074101.	1.2	1,185
25	Symmetry-Adapted Finite Strain Landau Theory Applied to KMnF3. Crystals, 2020, 10, 124.	1.0	7
26	Ca-doped rare earth perovskite materials for tailored exsolution of metal nanoparticles. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 1055-1070.	0.5	15
27	On the calculation of the bandgap of periodic solids with MGGA functionals using the total energy. Journal of Chemical Physics, 2019, 151, 161102.	1.2	10
28	Semilocal exchange-correlation potentials for solid-state calculations: Current status and future directions. Journal of Applied Physics, 2019, 126, .	1.1	41
29	Comparative study of the PBE and SCAN functionals: The particular case of alkali metals. Journal of Chemical Physics, 2019, 150, 164119.	1.2	16
30	Limitations of the DFTâ€“1/2 method for covalent semiconductors and transition-metal oxides. Physical Review B, 2019, 99, .	1.1	27
31	DFT calculations of energy dependent XPS valence band spectra. Journal of Electron Spectroscopy and Related Phenomena, 2019, 230, 1-9.	0.8	14
32	Partially Dissociated Water Dimers at the Waterâ€“Hematite Interface. ACS Energy Letters, 2019, 4, 390-396.	8.8	32
33	Nonlocal van der Waals functionals for solids: Choosing an appropriate one. Physical Review Materials, 2019, 3, .	0.9	65
34	Molecular Structure of Isocyanic Acid, HNCO, the Imide of Carbon Dioxide. Journal of Physical Chemistry A, 2018, 122, 3287-3292.	1.1	8
35	Calcium Doping Facilitates Water Dissociation in Magnesium Oxide. Advanced Sustainable Systems, 2018, 2, 1700096.	2.7	12
36	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

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37	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
38	Effects of electron-phonon coupling on absorption spectrum: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>K</mml:mi></mml:math> edge of hexagonal boron nitride. Physical Review B, 2018, 98, .	1.1	26
39	Orbital-free approximations to the kinetic-energy density in exchange-correlation MGGA functionals: Tests on solids. Journal of Chemical Physics, 2018, 149, 144105.	1.2	17
40	DFT calculations of solids in the ground state. , 2018, , 67-100.		2
41	Thermochemical Energy Storage: Calcium Doping Facilitates Water Dissociation in Magnesium Oxide (Adv. Sustainable Syst. 1/2018). Advanced Sustainable Systems, 2018, 2, 1870004.	2.7	0
42	Interplay of magnetism and transport in HoBi. Physical Review B, 2018, 98, .	1.1	19
43	Assessment of the GLLB-SC potential for solid-state properties and attempts for improvement. Physical Review Materials, 2018, 2, .	0.9	44
44	DFT study of the electronic properties and the cubic to tetragonal phase transition in RbCaF3. Physical Review Materials, 2018, 2, .	0.9	13
45	Density-gradient-free variable in exchange-correlation functionals for detecting inhomogeneities in the electron density. Physical Review Materials, 2018, 2, .	0.9	0
46	Local environment effects in the magnetic properties and electronic structure of disordered FePt. Physical Review B, 2017, 95, .	1.1	5
47	Finite-strain Landau theory applied to the high-pressure phase transition of lead titanate. Physical Review B, 2017, 95, .	1.1	10
48	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
49	Computational Study of Al and Sc NMR Shielding in Metallic ScTâ€²Al Heusler Phases. Journal of Physical Chemistry C, 2017, 121, 12398-12406.	1.5	5
50	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
51	NMR shieldings from density functional perturbation theory: GIPAW versus all-electron calculations. Journal of Chemical Physics, 2017, 146, 064115.	1.2	15
52	Computational Study of Ga NMR Shielding in Metallic Gallides. Journal of Physical Chemistry C, 2017, 121, 753-760.	1.5	16
53	On the importance of local orbitals using second energy derivatives for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" id="mml66" display="inline" overflow="scroll" altimg="si66.gif"><mml:mi>d</mml:mi></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" id="mml67" display="inline" overflow="scroll" altimg="si67.gif"><mml:mi>f</mml:mi></mml:math> electrons. Computer Physics Communications, 2017, 220, 230-238.	3.0	22
54	Simple way to apply nonlocal van der Waals functionals within all-electron methods. Physical Review B, 2017, 96, .	1.1	16

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55	Computational Study of Y NMR Shielding in Intermetallic Yttrium Compounds. Journal of Physical Chemistry C, 2017, 121, 28454-28461.	1.5	2
56	Spectromicroscopy of C60 and azafullerene C59N: Identifying surface adsorbed water. Scientific Reports, 2016, 6, 35605.	1.6	19
57	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
58	Co on Fe3O4(001): Towards precise control of surface properties. Journal of Chemical Physics, 2016, 144, 094704.	1.2	28
59	Transition from Reconstruction toward Thin Film on the (110) Surface of Strontium Titanate. Nano Letters, 2016, 16, 2407-2412.	4.5	28
60	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
61	Assessment of different basis sets and DFT functionals for the calculation of structural parameters, vibrational modes and ligand binding energies of Zr 4 O 2 (carboxylate) 12 clusters. Computational and Theoretical Chemistry, 2016, 1084, 162-168.	1.1	29
62	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
63	Theoretical and Experimental Study on the Optoelectronic Properties of Nb₃O₇(OH) and Nb₂O₅ Photoelectrodes. Journal of Physical Chemistry C, 2016, 120, 23329-23338.	1.5	22
64	<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	68
65	Evaluating eigensolver schemes within the density functional theory package WIEN2k. , 2016, , .		0
66	Magnetocrystalline anisotropy of FePt: A detailed view. Physical Review B, 2016, 94, .	1.1	41
67	Approximations to the exact exchange potential: KLI versus semilocal. Physical Review B, 2016, 94, .	1.1	14
68	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
69	woptic: Optical conductivity with Wannier functions and adaptive k-mesh refinement. Computer Physics Communications, 2016, 202, 1-11.	3.0	14
70	Ab initioperspective on the Mollwo-Ivey relation for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>F</mml:mi></mml:mrow></mml:math> centers in alkali halides. Physical Review B, 2015, 92, .	1.1	17
71	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><mml:m by Soft-X-Ray ARPES: Rhombohedral Lattice Distortion and its Effect. Physical Review Letters, 2015, 114, 237601.	2.9	38
72	Comparison between exact and semilocal exchange potentials: An all-electron study for solids. Physical Review B, 2015, 91, .	1.1	33

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73	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
74	Selective Area Band Engineering of Graphene using Cobalt-Mediated Oxidation. Scientific Reports, 2015, 5, 15380.	1.6	6
75	NMR Shielding in Metals Using the Augmented Plane Wave Method. Journal of Physical Chemistry C, 2015, 119, 19390-19396.	1.5	30
76	Understanding of ³³S NMR Shielding in Inorganic Sulfides and Sulfates. Journal of Physical Chemistry C, 2015, 119, 731-740.	1.5	20
77	Electrocoloration of donor-doped lead zirconate titanate under DC field stress. Solid State Ionics, 2015, 281, 49-59.	1.3	10
78	How Close Are the Slater and Becke–Roussel Potentials in Solids?. Journal of Chemical Theory and Computation, 2015, 11, 4717-4726.	2.3	17
79	Subsurface cation vacancy stabilization of the magnetite (001) surface. Science, 2014, 346, 1215-1218.	6.0	222
80	Nonmagnetic and ferromagnetic fcc cerium studied with one-electron methods. Physical Review B, 2014, 89, .	1.1	13
81	Dependence of Magnetic Anisotropy Energy on c/a Ratio of X₂Fe₁₄B (X = Y, Pr, Dy). IEEE Transactions on Magnetics, 2014, 50, 1-4.	1.2	8
82	Calculating NMR chemical shifts using the augmented plane-wave method. Physical Review B, 2014, 89, .	1.1	39
83	DFT Study of the Role of Al³⁺ in the Fast Ion-Conductor Li_{7–3x}Al³⁺_xLa₃Zr₂O₁₂ Garnet. Chemistry of Materials, 2014, 26, 2617-2623.	8.0	108
84	Predicted topological phase transition in the SmS Kondo insulator under pressure. Physical Review B, 2014, 89, .	1.1	29
85	Quantized electronic fine structure with large anisotropy in ferromagnetic Fe films. Physical Review B, 2014, 90, .	1.1	2
86	Fully Consistent Finite-Strain Landau Theory for High-Pressure Phase Transitions. Physical Review X, 2014, 4, .	2.8	8
87	<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
88	Cluster Nucleation and Growth from a Highly Supersaturated Adatom Phase: Silver on Magnetite. ACS Nano, 2014, 8, 7531-7537.	7.3	51
89	Assessment of DFT functionals with NMR chemical shifts. Physical Review B, 2013, 87, .	1.1	72
90	Structural, Spectroscopic, and Computational Studies on Tl₄Si₅O₁₂: A Microporous Thallium Silicate. Inorganic Chemistry, 2013, 52, 8941-8949.	1.9	5

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91	Room-temperature spin-spiral multiferroicity in high-pressure cupric oxide. Nature Communications, 2013, 4, 2511.	5.8	76
92	Oxide Heterostructures for Efficient Solar Cells. Physical Review Letters, 2013, 110, 078701.	2.9	113
93	Strain-induced topological insulator phase transition in HgSe. Physical Review B, 2013, 87, .	1.1	33
94	Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>t</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mi>g</mml:mi></mml:mrow></mml:msu 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 /><mml:mn>2</mml:mn></mml:msub></mml:math>/Nb<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
95	<mml:mn>2</mml:mn></mml:msub></mml:math>Nb<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	18
96	Carbon monoxide-induced adatom sintering in a Pdâ€“Fe3O4 model catalyst. Nature Materials, 2013, 12, 724-728.	13.3	249
97	Intrinsic uncertainty on ab initio phase diagram and compound formation energy calculations: BCC Moâ€“Fe as a test case. Physica Status Solidi (B): Basic Research, 2013, 250, 77-85.	0.7	7
98	Conducting states caused by a surface electric dipole in CrN(001) very thin films. Physical Review B, 2013, 87, .	1.1	12
99	Hybrid functionals for solids with an optimized Hartreeâ€“Fock mixing parameter. Journal of Physics Condensed Matter, 2013, 25, 435503.	0.7	74
100	Theoretical Investigation of the Magnetic Exchange Interactions in Copper(II) Oxides under Chemical and Physical Pressures. Scientific Reports, 2012, 2, 759.	1.6	59
101	Electronic structure of CrN: A comparison between different exchange correlation potentials. Physical Review B, 2012, 85, .	1.1	42
102	Calculating energy loss spectra of NiO: Advantages of the modified Becke-Johnson potential. Physical Review B, 2012, 85, .	1.1	28
103	Application of screened hybrid functionals to the bulk transition metals Rh, Pd, and Pt. Physical Review B, 2012, 86, .	1.1	24
104	Improving the modified Becke-Johnson exchange potential. Physical Review B, 2012, 85, .	1.1	552
105	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
106	Accounting for spin fluctuations beyond local spin density approximation in the density functional theory. Physical Review B, 2012, 86, .	1.1	43
107	Adsorption of small gold clusters on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>h</mml:mi></mml:math>-BN/Rh(111) nanomesh. Physical Review B, 2012, 86, .	1.1	24
108	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

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109	Origin of NMR shielding in fluorides. Physical Review B, 2012, 85, .	1.1	30
110	Calculations of NMR chemical shifts with APW-based methods. Physical Review B, 2012, 85, .	1.1	41
111	Ab Initio Study of Lattice Site Occupancies in Binary Sigma Phases Using a Single-Site Mean Field Model. Applied Sciences (Switzerland), 2012, 2, 654-668.	1.3	11
112	CeO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>/Pt(111) interface studied using first-principles density functional theory calculations. Physical Review B, 2011, 84, .	1.1	27
113	Configurational thermodynamics of the Fe-CrÏƒ phase. Physical Review B, 2011, 84, .	1.1	16
114	Ab initio-based mean-field theory of the site occupation in the Fe-Cr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Ïƒ</mml:mi></mml:mrow></mml:math>-phase. Physical Review B, 2011, 83, .	1.1	16
115	Comment on â€œHigh-TcFerroelectricity Emerging from Magnetic Degeneracy in Cupric Oxideâ€. Physical Review Letters, 2011, 107, 239701; discussion 239702.	2.9	9
116	Merits and limits of the modified Becke-Johnson exchange potential. Physical Review B, 2011, 83, .	1.1	743
117	Construction of an optimal GGA functional for molecules and solids. Physical Review B, 2011, 83, .	1.1	84
118	Implementation of screened hybrid functionals based on the Yukawa potential within the LAPW basis set. Physical Review B, 2011, 83, .	1.1	159
119	Adsorption of gold atoms on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>h</mml:mi></mml:math>-BN/Rh(111) nanomesh. Physical Review B, 2011, 84, .	1.1	25
120	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
121	Quantum oscillations of the superconductor LaRu2P2: Comparable mass enhancementÎ»â‰ˆ1in Ru and Fe phosphides. Physical Review B, 2011, 84, .	1.1	11
122	The Atomic Site Occupancies in the Fe-Cr Ïƒ-Phase. Solid State Phenomena, 2011, 170, 13-16.	0.3	3
123	Iterative diagonalization in augmented plane wave based methods in electronic structure calculations. Journal of Computational Physics, 2010, 229, 453-460.	1.9	21
124	Bulk vs. surface effects in ARPES experiment from La2/3Sr1/3MnO3 thin films. Journal of Electron Spectroscopy and Related Phenomena, 2010, 181, 63-69.	0.8	9
125	Calculations of MÃ¶ssbauer parameters in solids by DFT bandstructure calculations. Journal of Physics: Conference Series, 2010, 217, 012009.	0.3	25
126	Ab initiostudy of stabilization of the misfit layer compound<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mtext>PbS</mml:mtex Physical Review B, 2010, 82, .	1.1	16

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127	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:m 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
128	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></mml:mr Physical Review B, 2010, 82, .	1.1	74
129	Epitaxial growth of hexagonal boron nitride on Ag(111). Physical Review B, 2010, 82, .	1.1	75
130	Systematic investigation of a family of gradient-dependent functionals for solids. Physical Review B, 2010, 81, .	1.1	36
131	Towards efficient band structure and effective mass calculations for III-V direct band-gap semiconductors. Physical Review B, 2010, 82, .	1.1	279
132	Polarization-Dependent Raman Characterization of Stibnite (Sb[sub 2]S[sub 3]). AIP Conference Proceedings, 2010, , .	0.3	30
133	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
134	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
135	Short-range magnetic order and temperature-dependent properties of cupric oxide. Journal of Physics Condensed Matter, 2010, 22, 045502.	0.7	35
136	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: 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>c Physical Review B, 2010, 82, .	1.1	44
137	Electronic structure of solids with WIEN2k. Molecular Physics, 2010, 108, 3147-3166.	0.8	133
138	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:m transparent conductive oxides. Physical Review B, 2009, 79, .	1.1	76
139	Insight into the performance of GGA functionals for solid-state calculations. Physical Review B, 2009, 80, .	1.1	72
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