Peter Bláha

List of Articles by Year in descending order

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345 peer-reviewed articles	36,292 peer-reviewed citations	7348 76 peer-reviewed h-index	512253 3.84 score
365 documents	38947 doc citations	8932 79 h-index	37342 citing authors

#	Article	IF	Citations
1	How to verify the precision of density-functional-theory implementations via reproducible and universal workflows. Nature Reviews Physics, 2024, 6, 45-58.	31.5	84
2	Nonzero spontaneous electric polarization in metals: novel predictive methods and applications. Scientific Reports, 2024, 14, .	2.7	4
3	Engineering surface dipoles on mixed conducting oxides with ultra-thin oxide decoration layers. Nature Communications, 2024, 15, .	10.8	39
4	CoTeO4 – a wide-bandgap material adopting the dirutile structure type. Materials Advances, 2024, 5, 3001-3013.	3.8	7
5	Electronic and ionic effects of sulphur and other acidic adsorbates on the surface of an SOFC cathode material. Journal of Materials Chemistry A, 2023, 11, 7213-7226.	6.7	22
6	Large Topological Hall Effect and Spiral Magnetic Order in the Weyl Semimetal SmAlSi. Physical Review X, 2023, 13, .	7.9	42
7	DFT + U Simulation of the X-ray Absorption Near-Edge Structure of Bulk UO2 and PuO2. Journal of Physical Chemistry C, 2023, 127, 17994-18000.	2.3	7
8	Origin of the success of mGGAs for bandgaps. Journal of Chemical Physics, 2023, 159, .	2.2	6
9	WloopPHI: A tool for ab initio characterization of Weyl semimetals. Computer Physics Communications, 2022, 270, 108147.	2.8	8
10	Length-Gauge Optical Matrix Elements in WIEN2k. Computation, 2022, 10, 22.	1.5	4
11	CO Adsorption and Disproportionation on Smooth and Defect-Rich Ir(111). Journal of Physical Chemistry C, 2022, 126, 6578-6589.	2.3	10
12	Implementation of self-consistent MGGA functionals in augmented plane wave based methods. Physical Review B, 2022, 105, .	2.4	17
13	What is the optimal mGGA exchange functional for solids?. Journal of Chemical Physics, 2022, 157, .	2.2	18
14	Correct and Accurate Polymorphic Energy Ordering of Transition-Metal Monoxides Obtained from Semilocal and Onsite-Hybrid Exchange-Correlation Approximations. Journal of Physical Chemistry C, 2022, 126, 14650-14660.	2.3	5
15	Perturbation approach to ab initio effective mass calculations. Computer Physics Communications, 2021, 261, 107648.	2.8	42
16	Elucidating the formation and active state of Cu co-catalysts for photocatalytic hydrogen evolution. Journal of Materials Chemistry A, 2021, 9, 21958-21971.	6.7	36
17	Giant spontaneous Hall effect in a nonmagnetic Weyl–Kondo semimetal. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	5.2	123
18	Light emission from direct band gap germanium containing split-interstitial defects. Physical Review B, 2021, 103, .	2.4	17

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19	First-principles self-consistent phonon approach to the study of the vibrational properties and structural phase transition of BaTiO3. Physical Review B, 2021, 103, .	2.4	25
20	Efficient Band Structure Calculation of Two-Dimensional Materials from Semilocal Density Functionals. Journal of Physical Chemistry C, 2021, 125, 11206-11215.	2.3	33
21	Pristine quantum criticality in a Kondo semimetal. Science Advances, 2021, 7, .	8.1	17
22	Bandgap of two-dimensional materials: Thorough assessment of modern exchange–correlation functionals. Journal of Chemical Physics, 2021, 155, .	2.2	46
23	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.	1.3	1
24	Density analysis for estimating the degree of on-site correlation on transition-metal atoms in extended systems. Physical Review B, 2021, 104, .	2.4	1
25	Density Functional Theory Study of Metal and Metal-Oxide Nucleation and Growth on the Anatase TiO2(101) Surface. Computation, 2021, 9, 125.	1.5	6
26	Stress tensor in the linearized augmented plane wave method. Physical Review B, 2021, 104, .	2.4	3
27	Spin-resolved charge density and wavefunction refinements: the Mollynx/MoPro software. Acta Crystallographica Section A: Foundations and Advances, 2021, 77, C67-C68.	0.0	0
28	Measurement of electric quadrupole moment in neutron rich ^{131,132}I. European Physical Journal A, 2020, 56, .	1.7	1
29	Shortcomings of meta-GGA functionals when describing magnetism. Physical Review B, 2020, 102, .	2.4	50
30	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.	2.3	18
31	Modifying the Surface Structure of Perovskite-Based Catalysts by Nanoparticle Exsolution. Catalysts, 2020, 10, 268.	3.0	50
32	Local geometry around B atoms in B/Si(1 1 1) from polarized x-ray absorption spectroscopy. Journal of Physics Condensed Matter, 2020, 32, 045901.	1.6	1
33	WIEN2k: An APW+lo program for calculating the properties of solids. Journal of Chemical Physics, 2020, 152, .	2.2	2,543
34	Symmetry-Adapted Finite Strain Landau Theory Applied to KMnF3. Crystals, 2020, 10, 124.	1.8	7
35	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.	1.0	22
36	On the calculation of the bandgap of periodic solids with MGGA functionals using the total energy. Journal of Chemical Physics, 2019, 151, .	2.2	12

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37	Comparative study of the PBE and SCAN functionals: The particular case of alkali metals. Journal of Chemical Physics, 2019, 150, .	2.2	29
38	Limitations of the DFT–1/2 method for covalent semiconductors and transition-metal oxides. Physical Review B, 2019, 99, .	2.4	44
39	DFT calculations of energy dependent XPS valence band spectra. Journal of Electron Spectroscopy and Related Phenomena, 2019, 230, 1-9.	1.5	31
40	Partially Dissociated Water Dimers at the Water–Hematite Interface. ACS Energy Letters, 2019, 4, 390-396.	12.4	42
41	Nonlocal van der Waals functionals for solids: Choosing an appropriate one. Physical Review Materials, 2019, 3, .	1.8	95
42	Molecular Structure of Isocyanic Acid, HNCO, the Imide of Carbon Dioxide. Journal of Physical Chemistry A, 2018, 122, 3287-3292.	1.8	12
43	Calcium Doping Facilitates Water Dissociation in Magnesium Oxide. Advanced Sustainable Systems, 2018, 2, .	3.7	12
44	Atomic-Scale Structure of the Hematite α-Fe2O3(1$\bar{1}$02) “R-Cut” Surface. Journal of Physical Chemistry C, 2018, 122, 1657-1669.	2.3	125
45	Ordered Mesoporous TiO2 Gyroids: Effects of Pore Architecture and Nb-Doping on Photocatalytic Hydrogen Evolution under UV and Visible Irradiation. Advanced Energy Materials, 2018, 8, .	16.3	65
46	Effects of electron-phonon coupling on absorption spectrum: K edge of hexagonal boron nitride. Physical Review B, 2018, 98, .	2.4	56
47	Orbital-free approximations to the kinetic-energy density in exchange-correlation MGGA functionals: Tests on solids. Journal of Chemical Physics, 2018, 149, .	2.2	22
48	Interplay of magnetism and transport in HoBi. Physical Review B, 2018, 98, .	2.4	19
49	Assessment of the GLLB-SC potential for solid-state properties and attempts for improvement. Physical Review Materials, 2018, 2, .	1.8	61
50	DFT study of the electronic properties and the cubic to tetragonal phase transition in RbCaF3. Physical Review Materials, 2018, 2, .	1.8	19
51	Density-gradient-free variable in exchange-correlation functionals for detecting inhomogeneities in the electron density. Physical Review Materials, 2018, 2, .	1.8	0
52	Local environment effects in the magnetic properties and electronic structure of disordered FePt. Physical Review B, 2017, 95, .	2.4	6
53	Finite-strain Landau theory applied to the high-pressure phase transition of lead titanate. Physical Review B, 2017, 95, .	2.4	11
54	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.	1.8	180

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55	Computational Study of Al and Sc NMR Shielding in Metallic ScTT'Al Heusler Phases. Journal of Physical Chemistry C, 2017, 121, 12398-12406.	2.3	6
56	Investigation of the Optical and Excitonic Properties of the Visible Light-Driven Photocatalytic BiVO4 Material. Chemistry of Materials, 2017, 29, 3380-3386.	4.6	46
57	NMR shieldings from density functional perturbation theory: GIPAW versus all-electron calculations. Journal of Chemical Physics, 2017, 146, .	2.2	25
58	Computational Study of Ga NMR Shielding in Metallic Gallides. Journal of Physical Chemistry C, 2017, 121, 753-760.	2.3	17
59	On the importance of local orbitals using second energy derivatives for d and f electrons. Computer Physics Communications, 2017, 220, 230-238.	2.8	31
60	Simple way to apply nonlocal van der Waals functionals within all-electron methods. Physical Review B, 2017, 96, .	2.4	16
61	Computational Study of Y NMR Shielding in Intermetallic Yttrium Compounds. Journal of Physical Chemistry C, 2017, 121, 28454-28461.	2.3	2
62	Spectromicroscopy of C60 and azafullerene C59N: Identifying surface adsorbed water. Scientific Reports, 2016, 6, .	2.7	24
63	Rungs 1 to 4 of DFT Jacob's ladder: Extensive test on the lattice constant, bulk modulus, and cohesive energy of solids. Journal of Chemical Physics, 2016, 144, .	2.2	253
64	Co on Fe3O4(001): Towards precise control of surface properties. Journal of Chemical Physics, 2016, 144, .	2.2	31
65	Transition from Reconstruction toward Thin Film on the (110) Surface of Strontium Titanate. Nano Letters, 2016, 16, 2407-2412.	6.2	37
66	Band Gap Extraction from Individual Two-Dimensional Perovskite Nanosheets Using Valence Electron Energy Loss Spectroscopy. Journal of Physical Chemistry C, 2016, 120, 11170-11179.	2.3	39
67	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.	1.9	36
68	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.	5.2	134
69	Theoretical and Experimental Study on the Optoelectronic Properties of Nb3O7(OH) and Nb2O5 Photoelectrodes. Journal of Physical Chemistry C, 2016, 120, 23329-23338.	2.3	37
70	GWwith linearized augmented plane waves extended by high-energy local orbitals. Physical Review B, 2016, 93, .	2.4	80
71	Magnetocrystalline anisotropy of FePt: A detailed view. Physical Review B, 2016, 94, .	2.4	52
72	Approximations to the exact exchange potential: KLI versus semilocal. Physical Review B, 2016, 94, .	2.4	15

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73	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, .	26.1	1,536
74	woptic: Optical conductivity with Wannier functions and adaptive k-mesh refinement. Computer Physics Communications, 2016, 202, 1-11.	2.8	20
75	Ab initioperspective on the Mollwo-Ivey relation forFcenters in alkali halides. Physical Review B, 2015, 92, .	2.4	19
76	Fermi Surface of Three-DimensionalLa1−xSrxMnO3Explored by Soft-X-Ray ARPES: Rhombohedral Lattice Distortion and its Effect on Magnetoresistance. Physical Review Letters, 2015, 114, .	5.8	42
77	Comparison between exact and semilocal exchange potentials: An all-electron study for solids. Physical Review B, 2015, 91, .	2.4	43
78	Adsorption and incorporation of transition metals at the magnetiteFe3O4(001) surface. Physical Review B, 2015, 92, .	2.4	95
79	Selective Area Band Engineering of Graphene using Cobalt-Mediated Oxidation. Scientific Reports, 2015, 5, .	2.7	9
80	NMR Shielding in Metals Using the Augmented Plane Wave Method. Journal of Physical Chemistry C, 2015, 119, 19390-19396.	2.3	35
81	Understanding of 33S NMR Shielding in Inorganic Sulfides and Sulfates. Journal of Physical Chemistry C, 2015, 119, 731-740.	2.3	22
82	Electrocoloration of donor-doped lead zirconate titanate under DC field stress. Solid State Ionics, 2015, 281, 49-59.	2.6	11
83	How Close Are the Slater and Becke–Roussel Potentials in Solids?. Journal of Chemical Theory and Computation, 2015, 11, 4717-4726.	3.6	17
84	LEMS: application of the method to study the static quadrupole moment of the isomer in 179W. Zeitschrift Für Physik A, 2014, 358, 267-268.	0.3	0
85	Nonmagnetic and ferromagnetic fcc cerium studied with one-electron methods. Physical Review B, 2014, 89, .	2.4	16
86	Dependence of Magnetic Anisotropy Energy on c/a Ratio of X2Fe14B (X = Y, Pr, Dy). IEEE Transactions on Magnetics, 2014, 50, 1-4.	1.0	10
87	Calculating NMR chemical shifts using the augmented plane-wave method. Physical Review B, 2014, 89, .	2.4	46
88	DFT Study of the Role of Al3+ in the Fast Ion-Conductor Li7−3xAl3+xLa3Zr2O12 Garnet. Chemistry of Materials, 2014, 26, 2617-2623.	4.6	135
89	Predicted topological phase transition in the SmS Kondo insulator under pressure. Physical Review B, 2014, 89, .	2.4	29
90	Quantized electronic fine structure with large anisotropy in ferromagnetic Fe films. Physical Review B, 2014, 90, .	2.4	2

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91	Fully Consistent Finite-Strain Landau Theory for High-Pressure Phase Transitions. Physical Review X, 2014, 4, .	7.9	10
92	Fcenter in lithium fluoride revisited: Comparison of solid-state physics and quantum-chemistry approaches. Physical Review B, 2014, 89, .	2.4	53
93	Cluster Nucleation and Growth from a Highly Supersaturated Adatom Phase: Silver on Magnetite. ACS Nano, 2014, 8, 7531-7537.	11.5	57
94	Assessment of DFT functionals with NMR chemical shifts. Physical Review B, 2013, 87, .	2.4	84
95	Structural, Spectroscopic, and Computational Studies on Tl4Si5O12: A Microporous Thallium Silicate. Inorganic Chemistry, 2013, 52, 8941-8949.	3.4	7
96	Room-temperature spin-spiral multiferroicity in high-pressure cupric oxide. Nature Communications, 2013, 4, .	10.8	83
97	Oxide Heterostructures for Efficient Solar Cells. Physical Review Letters, 2013, 110, .	5.8	127
98	Strain-induced topological insulator phase transition in HgSe. Physical Review B, 2013, 87, .	2.4	39
99	Fet2gband dispersion and spin polarization in thin films of Fe3O4(0 0 1)/MgO(0 0 1): Half-metallicity of magnetite revisited. Physical Review B, 2013, 87, .	2.4	44
100	Electronic structure of KCa2Nb3O10as envisaged by density functional theory and valence electron energy loss spectroscopy. Physical Review B, 2013, 87, .	2.4	24
101	Carbon monoxide-induced adatom sintering in a Pd–Fe3O4 model catalyst. Nature Materials, 2013, 12, 724-728.	23.7	326
102	Intrinsic uncertainty on ab initio phase diagram and compound formation energy calculations: BCC Mo–Fe as a test case. Physica Status Solidi (B): Basic Research, 2013, 250, 77-85.	1.0	7
103	Conducting states caused by a surface electric dipole in CrN(001) very thin films. Physical Review B, 2013, 87, .	2.4	16
104	Hybrid functionals for solids with an optimized Hartree–Fock mixing parameter. Journal of Physics Condensed Matter, 2013, 25, 435503.	1.6	92
105	Theoretical Investigation of the Magnetic Exchange Interactions in Copper(II) Oxides under Chemical and Physical Pressures. Scientific Reports, 2012, 2, .	2.7	70
106	Electronic structure of CrN: A comparison between different exchange correlation potentials. Physical Review B, 2012, 85, .	2.4	50
107	Calculating energy loss spectra of NiO: Advantages of the modified Becke-Johnson potential. Physical Review B, 2012, 85, .	2.4	31
108	Application of screened hybrid functionals to the bulk transition metals Rh, Pd, and Pt. Physical Review B, 2012, 86, .	2.4	25

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109	Improving the modified Becke-Johnson exchange potential. Physical Review B, 2012, 85, .	2.4	869
110	Ferromagnetic insulating state in tensile-strained LaCoO3thin films from LDA+Ucalculations. Physical Review B, 2012, 85, .	2.4	72
111	Accounting for spin fluctuations beyond local spin density approximation in the density functional theory. Physical Review B, 2012, 86, .	2.4	50
112	Adsorption of small gold clusters on theh-BN/Rh(111) nanomesh. Physical Review B, 2012, 86, .	2.4	25
113	Three-Dimensional Electron Realm inVSe2by Soft-X-Ray Photoelectron Spectroscopy: Origin of Charge-Density Waves. Physical Review Letters, 2012, 109, .	5.8	176
114	Origin of NMR shielding in fluorides. Physical Review B, 2012, 85, .	2.4	33
115	Calculations of NMR chemical shifts with APW-based methods. Physical Review B, 2012, 85, .	2.4	48
116	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.	1.6	16
117	CeO2/Pt(111) interface studied using first-principles density functional theory calculations. Physical Review B, 2011, 84, .	2.4	33
118	Configurational thermodynamics of the Fe-Crσphase. Physical Review B, 2011, 84, .	2.4	16
119	Ab initio-based mean-field theory of the site occupation in the Fe-Crσ-phase. Physical Review B, 2011, 83, .	2.4	16
120	Comment on “High-TcFerroelectricity Emerging from Magnetic Degeneracy in Cupric Oxide”. Physical Review Letters, 2011, 107, .	5.8	9
121	Merits and limits of the modified Becke-Johnson exchange potential. Physical Review B, 2011, 83, .	2.4	1,034
122	Construction of an optimal GGA functional for molecules and solids. Physical Review B, 2011, 83, .	2.4	115
123	Implementation of screened hybrid functionals based on the Yukawa potential within the LAPW basis set. Physical Review B, 2011, 83, .	2.4	193
124	Adsorption of gold atoms on theh-BN/Rh(111) nanomesh. Physical Review B, 2011, 84, .	2.4	26
125	Spin-State Crossover and Hyperfine Interactions of Ferric Iron inMgSiO3Perovskite. Physical Review Letters, 2011, 106, .	5.8	160
126	Quantum oscillations of the superconductor LaRu2P2: Comparable mass enhancementλ≈1in Ru and Fe phosphides. Physical Review B, 2011, 84, .	2.4	14

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127	Iterative diagonalization in augmented plane wave based methods in electronic structure calculations. Journal of Computational Physics, 2010, 229, 453-460.	2.9	34
128	Bulk vs. surface effects in ARPES experiment from La2/3Sr1/3MnO3 thin films. Journal of Electron Spectroscopy and Related Phenomena, 2010, 181, 63-69.	1.5	10
129	Calculations of Mössbauer parameters in solids by DFT bandstructure calculations. Journal of Physics: Conference Series, 2010, 217, 012009.	0.2	25
130	Ab initiostudy of stabilization of the misfit layer compound(PbS)1.14TaS2. Physical Review B, 2010, 82, .	2.4	23
131	Understanding theL2,3x-ray absorption spectra of early3dtransition elements. Physical Review B, 2010, 82, .	2.4	141
132	Temperature and composition dependence of crystal structures and magnetic and electronic properties of the double perovskitesLa2−xSrxCoIrO6(0≤x≤2). Physical Review B, 2010, 82, .	2.4	86
133	Epitaxial growth of hexagonal boron nitride on Ag(111). Physical Review B, 2010, 82, .	2.4	82
134	Systematic investigation of a family of gradient-dependent functionals for solids. Physical Review B, 2010, 81, .	2.4	38
135	Towards efficient band structure and effective mass calculations for III-V direct band-gap semiconductors. Physical Review B, 2010, 82, .	2.4	322
136	Spin states and hyperfine interactions of iron in (Mg,Fe)SiO3 perovskite under pressure. Earth and Planetary Science Letters, 2010, 294, 19-26.	3.4	109
137	Ab initiostudy ofh−BNnanomeshes on Ru(001), Rh(111), and Pt(111). Physical Review B, 2010, 81, .	2.4	68
138	Short-range magnetic order and temperature-dependent properties of cupric oxide. Journal of Physics Condensed Matter, 2010, 22, 045502.	1.6	36
139	Cobalt spin states and hyperfine interactions inLaCoO3investigated byLDA+Ucalculations. Physical Review B, 2010, 82, .	2.4	49
140	Electronic structure of solids with WIEN2k. Molecular Physics, 2010, 108, 3147-3166.	1.1	192
141	Strong excitonic effects inCuAlO2delafossite transparent conductive oxides. Physical Review B, 2009, 79, .	2.4	86
142	Insight into the performance of GGA functionals for solid-state calculations. Physical Review B, 2009, 80, .	2.4	135
143	The small unit cell reconstructions of SrTiO3(111). Surface Science, 2009, 603, 2179-2187.	1.5	34
144	Density functional theory simulations of B K and N K NEXAFS spectra of h-BN/transition metal(111) interfaces. Journal of Physics Condensed Matter, 2009, 21, 104210.	1.6	23

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145	Accurate Band Gaps of Semiconductors and Insulators with a Semilocal Exchange-Correlation Potential. Physical Review Letters, 2009, 102, .	5.8	5,796
146	Calculation of the lattice constant of solids with semilocal functionals. Physical Review B, 2009, 79, .	2.4	815
147	Density functional calculations on the charge-ordered and valence-mixed modification ofYBaFe2O5. Physical Review B, 2009, 79, .	2.4	35
148	Force calculation for orbital-dependent potentials with FP-(L)APW+lo basis sets. Computer Physics Communications, 2008, 179, 784-790.	2.8	27
149	Bonding of hexagonal BN to transition metal surfaces: Anab initiodensity-functional theory study. Physical Review B, 2008, 78, .	2.4	165
150	Structure and stability ofCd2Nb2O7andCd2Ta2O7explored byab initiocalculations. Physical Review B, 2008, 78, .	2.4	49
151	Unraveling the structure of the h-BN/Rh(111) nanomesh withab initiocalculations. Journal of Physics Condensed Matter, 2008, 20, 064207.	1.6	42
152	Nuclear quadrupole interaction atS44cin the anatase and rutile modifications ofTiO2: Time-differential perturbed-angular-correlation measurements andab initiocalculations. Physical Review B, 2008, 77, .	2.4	28
153	PBE+Ucalculations of the Jahn-Teller effect inPrO2. Physical Review B, 2008, 77, .	2.4	40
154	Multiple instabilities inBi4Ti3O12: A ferroelectric beyond the soft-mode paradigm. Physical Review B, 2008, 77, .	2.4	62
155	Effects of three-dimensional band structure in angle- and spin-resolved photoemission from half-metallicLa2/3Sr1/3MnO3. Physical Review B, 2008, 77, .	2.4	32
156	Hidden surface states on pristine and H-passivated Ni(111): Angle-resolved photoemission and density-functional calculations. Physical Review B, 2008, 77, .	2.4	20
157	Influence of reconstruction on the surface state of Au(110). Physical Review B, 2008, 78, .	2.4	44
158	Origin of the light green color and electronic ground state ofLaCrO3. Physical Review B, 2008, 77, .	2.4	71
159	Structural vs electronic origin of renormalized band widths in TTF-TCNQ: An angular dependent NEXAFS study. Physical Review B, 2007, 76, .	2.4	14
160	Composite Behavior and Multidegeneracy in High-Pressure Phases of Cs and Rb. Physical Review Letters, 2007, 99, .	5.8	7
161	Deep multilayer relaxations on the Al(001) surface:Ab initioall-electron calculations. Physical Review B, 2007, 76, .	2.4	15
162	Spin-polarized standing waves at an electronically matched interface detected by Fermi-surface photoemission. Physical Review B, 2007, 75, .	2.4	6

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163	Band gap calculations with Becke–Johnson exchange potential. Journal of Physics Condensed Matter, 2007, 19, 196208.	1.6	292
164	Advances in Structural Analysis of Fluoroaluminates Using DFT Calculations of 27Al Electric Field Gradients. Journal of Physical Chemistry A, 2007, 111, 11873-11884.	1.8	33
165	Mixed PbFBr1−xIxcrystals: structural and spectroscopic investigations. Journal of Physics Condensed Matter, 2007, 19, 036214.	1.6	5
166	Electronic Structure and Optical Properties of AFeO2(A = Ag, Cu) within GGA Calculations. Chemistry of Materials, 2007, 19, 634-640.	4.6	104
167	Ising-type behavior in the antiferromagnetic phase ofBaCoO3from first principles. Physical Review B, 2007, 76, .	2.4	10
168	Performance on molecules, surfaces, and solids of the Wu-Cohen GGA exchange-correlation energy functional. Physical Review B, 2007, 75, .	2.4	354
169	Single-Layer Model of the Hexagonal Boron Nitride Nanomesh on the Rh(111) Surface. Physical Review Letters, 2007, 98, .	5.8	148
170	Boron Nitride Nanomesh: Functionality from a Corrugated Monolayer. Angewandte Chemie - International Edition, 2007, 46, 5115-5119.	11.6	219
171	Boron Nitride Nanomesh: Functionality from a Corrugated Monolayer. Angewandte Chemie, 2007, 119, 5207-5211.	0.9	23
172	The electronic structure and crystal field of RPt3Si (R=Pr, Nd, Sm) compounds. Physica B: Condensed Matter, 2007, 400, 114-118.	2.2	5
173	Hybrid exchange-correlation energy functionals for strongly correlated electrons: Applications to transition-metal monoxides. Physical Review B, 2006, 74, .	2.4	352
174	27Al NMR experiments and quadrupolar parameter ab initio calculations: Crystallographic structure refinement of β-Ba3AlF9. Chemical Physics Letters, 2006, 424, 321-326.	2.0	21
175	Possible non-collinear magnetic configurations in BaCoO3. Physica B: Condensed Matter, 2006, 378-380, 556-557.	2.2	2
176	Electronic quasiparticles and evolution of Fermi level spin states in thin magnetic layers. Surface Science, 2006, 600, 3912-3916.	1.5	3
177	Structure and properties of CoMnSb in the context of half-metallic ferromagnetism. Physical Review B, 2006, 74, .	2.4	59
178	Chemical bonding based on charge density calculations for solids. Acta Crystallographica Section A: Foundations and Advances, 2005, 61, c427-c427.	0.2	0
179	Structural investigations of β-CaAlF5 by coupling powder XRD, NMR, EPR and spectroscopic parameter calculations. Journal of Solid State Chemistry, 2005, 178, 3655-3661.	2.4	28
180	Bandstructure study of magnetic and orbital order in. Journal of Magnetism and Magnetic Materials, 2005, 290-291, 349-352.	2.1	2

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181	Experimental and theoretical bond critical point properties for model electron density distributions for earth materials. Physics and Chemistry of Minerals, 2005, 32, 114-125.	0.8	14
182	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.	0.8	73
183	Ab initio electronic structure of rare earth orthoferrites. Journal of Magnetism and Magnetic Materials, 2005, 290-291, 396-399.	2.1	20
184	Mössbauer study of LaNiSn and NdNiSn compounds and their deuterides. Journal of Radioanalytical and Nuclear Chemistry, 2005, 266, 553-556.	1.1	2
185	Crystal structure prediction with WIEN2k. Acta Crystallographica Section A: Foundations and Advances, 2005, 61, c19-c19.	0.2	0
186	Comment on “Taming multiple valency with density functionals: A case study of defective ceria”. Physical Review B, 2005, 72, .	2.4	92
187	Comparison of empirical bond-valence and first-principles energy calculations for a complex structural instability. Physical Review B, 2005, 72, .	2.4	27
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