Peter Blaha

List of Publications by Year in Descending Order

345 papers	27,243 citations	73 h-index	158 g-index
367 ext. papers	30,291 ext. citations	4 avg, IF	7.25 L-index

#	Paper	IF	Citations
345	Length-Gauge Optical Matrix Elements in WIEN2k. *Computation*, **2022**, 10, 22	2.2	0
344	WloopPHI: A tool for ab initio characterization of Weyl semimetals. *Computer Physics Communications*, **2022**, 270, 108147	4.2	0
343	CO Adsorption and Disproportionation on Smooth and Defect-Rich Ir(111).. *Journal of Physical Chemistry C*, **2022**, 126, 6578-6589	3.8	1
342	Density Functional Theory Study of Metal and Metal-Oxide Nucleation and Growth on the Anatase TiO2(101) Surface. *Computation*, **2021**, 9, 125	2.2	0
341	First-principles self-consistent phonon approach to the study of the vibrational properties and structural phase transition of BaTiO3. *Physical Review B*, **2021**, 103,	3.3	3
340	Efficient Band Structure Calculation of Two-Dimensional Materials from Semilocal Density Functionals. *Journal of Physical Chemistry C*, **2021**, 125, 11206-11215	3.8	2
339	Pristine quantum criticality in a Kondo semimetal. *Science Advances*, **2021**, 7,	14.3	2
338	Perturbation approach to ab initio effective mass calculations. *Computer Physics Communications*, **2021**, 261, 107648	4.2	5
337	Elucidating the formation and active state of Cu co-catalysts for photocatalytic hydrogen evolution. *Journal of Materials Chemistry A*, **2021**, 9, 21958-21971	13	3
336	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,	11.5	12
335	Light emission from direct band gap germanium containing split-interstitial defects. *Physical Review B*, **2021**, 103,	3.3	4
334	Bandgap of two-dimensional materials: Thorough assessment of modern exchange-correlation functionals. *Journal of Chemical Physics*, **2021**, 155, 104103	3.9	4
333	Te 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	3.1	0
332	Modifying the Surface Structure of Perovskite-Based Catalysts by Nanoparticle Exsolution. *Catalysts*, **2020**, 10, 268	4	18
331	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	1.8	1
330	WIEN2k: An APW+lo program for calculating the properties of solids. *Journal of Chemical Physics*, **2020**, 152, 074101	3.9	408
329	Symmetry-Adapted Finite Strain Landau Theory Applied to KMnF3. *Crystals*, **2020**, 10, 124	2.3	5

328	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	1.8	7
327	Measurement of electric quadrupole moment in neutron rich (^{131,132})I. *European Physical Journal A*, **2020**, 56, 1	2.5	
326	Shortcomings of meta-GGA functionals when describing magnetism. *Physical Review B*, **2020**, 102,	3.3	9
325	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	3.8	5
324	Semilocal exchange-correlation potentials for solid-state calculations: Current status and future directions. *Journal of Applied Physics*, **2019**, 126, 110902	2.5	21
323	Comparative study of the PBE and SCAN functionals: The particular case of alkali metals. *Journal of Chemical Physics*, **2019**, 150, 164119	3.9	11
322	Limitations of the DFT1/2 method for covalent semiconductors and transition-metal oxides. *Physical Review B*, **2019**, 99,	3.3	15
321	On the calculation of the bandgap of periodic solids with MGGA functionals using the total energy. *Journal of Chemical Physics*, **2019**, 151, 161102	3.9	5
320	Nonlocal van der Waals functionals for solids: Choosing an appropriate one. *Physical Review Materials*, **2019**, 3,	3.2	41
319	DFT calculations of energy dependent XPS valence band spectra. *Journal of Electron Spectroscopy and Related Phenomena*, **2019**, 230, 1-9	1.7	8
318	Partially Dissociated Water Dimers at the Water–Hematite Interface. *ACS Energy Letters*, **2019**, 4, 390-396	20.1	25
317	Molecular Structure of Isocyanic Acid, HNCO, the Imide of Carbon Dioxide. *Journal of Physical Chemistry A*, **2018**, 122, 3287-3292	2.8	5
316	Interplay of magnetism and transport in HoBi. *Physical Review B*, **2018**, 98,	3.3	8
315	Assessment of the GLLB-SC potential for solid-state properties and attempts for improvement. *Physical Review Materials*, **2018**, 2,	3.2	29
314	DFT study of the electronic properties and the cubic to tetragonal phase transition in RbCaF3. *Physical Review Materials*, **2018**, 2,	3.2	8
313	Calcium Doping Facilitates Water Dissociation in Magnesium Oxide. *Advanced Sustainable Systems*, **2018**, 2, 1700096	5.9	12
312	Atomic-Scale Structure of the Hematite –FeO(11 02) "R-Cut" Surface. *Journal of Physical Chemistry C*, **2018**, 122, 1657-1669	3.8	59
311	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, 1802566	21.8	32

310	Effects of electron-phonon coupling on absorption spectrum: K edge of hexagonal boron nitride. *Physical Review B*, **2018**, 98,	3.3	15
309	Orbital-free approximations to the kinetic-energy density in exchange-correlation MGGA functionals: Tests on solids. *Journal of Chemical Physics*, **2018**, 149, 144105	3.9	14
308	DFT calculations of solids in the ground state **2018**, 67-100		0
307	Thermochemical Energy Storage: Calcium Doping Facilitates Water Dissociation in Magnesium Oxide (Adv. Sustainable Syst. 1/2018). *Advanced Sustainable Systems*, **2018**, 2, 1870004	5.9	
306	Local environment effects in the magnetic properties and electronic structure of disordered FePt. *Physical Review B*, **2017**, 95,	3.3	5
305	Finite-strain Landau theory applied to the high-pressure phase transition of lead titanate. *Physical Review B*, **2017**, 95,	3.3	10
304	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	2.8	91
303	Computational Study of Al and Sc NMR Shielding in Metallic ScTT?Al Heusler Phases. *Journal of Physical Chemistry C*, **2017**, 121, 12398-12406	3.8	4
302	Investigation of the Optical and Excitonic Properties of the Visible Light-Driven Photocatalytic BiVO4 Material. *Chemistry of Materials*, **2017**, 29, 3380-3386	9.6	31
301	NMR shieldings from density functional perturbation theory: GIPAW versus all-electron calculations. *Journal of Chemical Physics*, **2017**, 146, 064115	3.9	12
300	Computational Study of Ga NMR Shielding in Metallic Gallides. *Journal of Physical Chemistry C*, **2017** , 121, 753-760	3.8	12
299	DFT Calculations for Real Solids **2017**, 227-259		3
298	On the importance of local orbitals using second energy derivatives for d and f electrons. *Computer Physics Communications*, **2017**, 220, 230-238	4.2	12
297	Simple way to apply nonlocal van der Waals functionals within all-electron methods. *Physical Review B*, **2017**, 96,	3.3	14
296	Computational Study of Y NMR Shielding in Intermetallic Yttrium Compounds. *Journal of Physical Chemistry C*, **2017**, 121, 28454-28461	3.8	1
295	Theoretical and Experimental Study on the Optoelectronic Properties of Nb3O7(OH) and Nb2O5 Photoelectrodes. *Journal of Physical Chemistry C*, **2016**, 120, 23329-23338	3.8	16
294	GW with linearized augmented plane waves extended by high-energy local orbitals. *Physical Review B*, **2016**, 93,	3.3	49
293	Magnetocrystalline anisotropy of FePt: A detailed view. *Physical Review B*, **2016**, 94,	3.3	29

292	Approximations to the exact exchange potential: KLI versus semilocal. *Physical Review B*, **2016**, 94,	3.3	13
291	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
290	woptic: Optical conductivity with Wannier functions and adaptive k-mesh refinement. *Computer Physics Communications*, **2016**, 202, 1-11	4.2	10
289	Spectromicroscopy of C and azafullerene CN: Identifying surface adsorbed water. *Scientific Reports*, **2016**, 6, 35605	4.9	9
288	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, 204120	3.9	142
287	Co on Fe3O4(001): Towards precise control of surface properties. *Journal of Chemical Physics*, **2016**, 144, 094704	3.9	24
286	Transition from Reconstruction toward Thin Film on the (110) Surface of Strontium Titanate. *Nano Letters*, **2016**, 16, 2407-12	11.5	25
285	Band Gap Extraction from Individual Two-Dimensional Perovskite Nanosheets Using Valence Electron Energy Loss Spectroscopy. *Journal of Physical Chemistry C*, **2016**, 120, 11170-11179	3.8	29
284	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	2	22
283	Dual role of CO in the stability of subnano Pt clusters at the Fe3O4(001) surface. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 8921-6	11.5	85
282	Electrocoloration of donor-doped lead zirconate titanate under DC field stress. *Solid State Ionics*, **2015**, 281, 49-59	3.3	7
281	How close are the Slater and Becke-Roussel potentials in solids?. *Journal of Chemical Theory and Computation*, **2015**, 11, 4717-26	6.4	15
280	Ab initio perspective on the Mollwo-Ivey relation for F centers in alkali halides. *Physical Review B*, **2015**, 92,	3.3	13
279	Fermi Surface of Three-Dimensional La(1-x)Sr(x)MnO3 Explored by Soft-X-Ray ARPES: Rhombohedral Lattice Distortion and its Effect on Magnetoresistance. *Physical Review Letters*, **2015**, 114, 237601	7.4	31
278	Comparison between exact and semilocal exchange potentials: An all-electron study for solids. *Physical Review B*, **2015**, 91,	3.3	25
277	Adsorption and incorporation of transition metals at the magnetite Fe3O4(001) surface. *Physical Review B*, **2015**, 92,	3.3	61
276	Selective Area Band Engineering of Graphene using Cobalt-Mediated Oxidation. *Scientific Reports*, **2015**, 5, 15380	4.9	6
275	NMR Shielding in Metals Using the Augmented Plane Wave Method. *Journal of Physical Chemistry C*, **2015**, 119, 19390-19396	3.8	23

274	Understanding of 33S NMR Shielding in Inorganic Sulfides and Sulfates. *Journal of Physical Chemistry C*, **2015**, 119, 731-740	3.8	18
273	Calculating NMR chemical shifts using the augmented plane-wave method. *Physical Review B*, **2014**, 89,	3.3	31
272	DFT Study of the Role of Al in the Fast Ion-Conductor Li Al LaZrO Garnet. *Chemistry of Materials*, **2014**, 26, 2617-2623	9.6	80
271	Predicted topological phase transition in the SmS Kondo insulator under pressure. *Physical Review B*, **2014**, 89,	3.3	25
270	Quantized electronic fine structure with large anisotropy in ferromagnetic Fe films. *Physical Review B*, **2014**, 90,	3.3	2
269	Fully Consistent Finite-Strain Landau Theory for High-Pressure Phase Transitions. *Physical Review X*, **2014**, 4,	9.1	7
268	F center in lithium fluoride revisited: Comparison of solid-state physics and quantum-chemistry approaches. *Physical Review B*, **2014**, 89,	3.3	36
267	Cluster nucleation and growth from a highly supersaturated adatom phase: silver on magnetite. *ACS Nano*, **2014**, 8, 7531-7	16.7	43
266	Subsurface cation vacancy stabilization of the magnetite (001) surface. *Science*, **2014**, 346, 1215-8	33.3	181
265	Nonmagnetic and ferromagnetic fcc cerium studied with one-electron methods. *Physical Review B*, **2014**, 89,	3.3	11
264	Dependence of Magnetic Anisotropy Energy on c/a Ratio of X2Fe14B (X = Y, Pr, Dy). *IEEE Transactions on Magnetics*, **2014**, 50, 1-4	2	7
263	Assessment of DFT functionals with NMR chemical shifts. *Physical Review B*, **2013**, 87,	3.3	58
262	Structural, spectroscopic, and computational studies on Tl4Si5O12: a microporous thallium silicate. *Inorganic Chemistry*, **2013**, 52, 8941-9	5.1	4
261	Room-temperature spin-spiral multiferroicity in high-pressure cupric oxide. *Nature Communications*, **2013**, 4, 2511	17.4	61
260	Oxide heterostructures for efficient solar cells. *Physical Review Letters*, **2013**, 110, 078701	7.4	92
259	Strain-induced topological insulator phase transition in HgSe. *Physical Review B*, **2013**, 87,	3.3	30
258	Fe t2g band 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,	3.3	34
257	Electronic structure of KCa2Nb3O10 as envisaged by density functional theory and valence electron energy loss spectroscopy. *Physical Review B*, **2013**, 87,	3.3	15

256	Carbon monoxide-induced adatom sintering in a Pd-Fe3O4 model catalyst. *Nature Materials*, **2013**, 12, 724-8	27	191
255	Intrinsic uncertainty on ab initio phase diagram and compound formation energy calculations: BCC Mo□e as a test case. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 77-85	1.3	6
254	Conducting states caused by a surface electric dipole in CrN(001) very thin films. *Physical Review B*, **2013**, 87,	3.3	11
253	Hybrid functionals for solids with an optimized Hartree-Fock mixing parameter. *Journal of Physics Condensed Matter*, **2013**, 25, 435503	1.8	55
252	Application of screened hybrid functionals to the bulk transition metals Rh, Pd, and Pt. *Physical Review B*, **2012**, 86,	3.3	20
251	Improving the modified Becke-Johnson exchange potential. *Physical Review B*, **2012**, 85,	3.3	383
250	Ferromagnetic insulating state in tensile-strained LaCoO3 thin films from LDA + U calculations. *Physical Review B*, **2012**, 85,	3.3	61
249	Accounting for spin fluctuations beyond local spin density approximation in the density functional theory. *Physical Review B*, **2012**, 86,	3.3	38
248	Adsorption of small gold clusters on the h-BN/Rh(111) nanomesh. *Physical Review B*, **2012**, 86,	3.3	20
247	Three-dimensional electron realm in VSe2 by soft-x-ray photoelectron spectroscopy: origin of charge-density waves. *Physical Review Letters*, **2012**, 109, 086401	7.4	102
246	Origin of NMR shielding in fluorides. *Physical Review B*, **2012**, 85,	3.3	27
245	Calculations of NMR chemical shifts with APW-based methods. *Physical Review B*, **2012**, 85,	3.3	39
244	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	2.6	9
243	Quantum Oscillations in Ultra Pure PtSn4. *Solid State Phenomena*, **2012**, 194, 88-91	0.4	5
242	Theoretical investigation of the magnetic exchange interactions in copper(II) oxides under chemical and physical pressures. *Scientific Reports*, **2012**, 2, 759	4.9	51
241	Electronic structure of CrN: A comparison between different exchange correlation potentials. *Physical Review B*, **2012**, 85,	3.3	38
240	Calculating energy loss spectra of NiO: Advantages of the modified Becke-Johnson potential. *Physical Review B*, **2012**, 85,	3.3	25
239	Configurational thermodynamics of the Fe-Cr □phase. *Physical Review B*, **2011**, 84,	3.3	15

238	Ab initio-based mean-field theory of the site occupation in the Fe-Cr phase. *Physical Review B*, **2011**, 83,	3.3	15
237	Comment on "High-Tc ferroelectricity emerging from magnetic degeneracy in cupric oxide". *Physical Review Letters*, **2011**, 107, 239701; discussion 239702	7.4	9
236	Merits and limits of the modified Becke-Johnson exchange potential. *Physical Review B*, **2011**, 83,	3.3	584
235	Construction of an optimal GGA functional for molecules and solids. *Physical Review B*, **2011**, 83,	3.3	71
234	Implementation of screened hybrid functionals based on the Yukawa potential within the LAPW basis set. *Physical Review B*, **2011**, 83,	3.3	121
233	CeO2/Pt(111) interface studied using first-principles density functional theory calculations. *Physical Review B*, **2011**, 84,	3.3	25
232	Adsorption of gold atoms on the h-BN/Rh(111) nanomesh. *Physical Review B*, **2011**, 84,	3.3	22
231	Spin-state crossover and hyperfine interactions of ferric iron in MgSiO(3) perovskite. *Physical Review Letters*, **2011**, 106, 118501	7.4	121
230	Quantum oscillations of the superconductor LaRu2P2: Comparable mass enhancement in Ru and Fe phosphides. *Physical Review B*, **2011**, 84,	3.3	8
229	The Atomic Site Occupancies in the Fe-Cr Phase. *Solid State Phenomena*, **2011**, 170, 13-16	0.4	3
228	Calculations of Mssbauer parameters in solids by DFT bandstructure calculations. *Journal of Physics: Conference Series*, **2010**, 217, 012009	0.3	21
227	Ab initio study of stabilization of the misfit layer compound (PbS)1.14TaS2. *Physical Review B*, **2010**, 82,	3.3	11
226	Understanding the L2,3 x-ray absorption spectra of early 3d transition elements. *Physical Review B*, **2010**, 82,	3.3	103
225	Temperature and composition dependence of crystal structures and magnetic and electronic properties of the double perovskites La2SrxCoIrO6 (0). *Physical Review B*, **2010**, 82,	3.3	58
224	Epitaxial growth of hexagonal boron nitride on Ag(111). *Physical Review B*, **2010**, 82,	3.3	69
223	Systematic investigation of a family of gradient-dependent functionals for solids. *Physical Review B*, **2010**, 81,	3.3	35
222	Towards efficient band structure and effective mass calculations for III-V direct band-gap semiconductors. *Physical Review B*, **2010**, 82,	3.3	239
221	Polarization-Dependent Raman Characterization of Stibnite (Sb2S3) **2010**,		18

220	Spin states and hyperfine interactions of iron in (Mg,Fe)SiO3 perovskite under pressure. *Earth and Planetary Science Letters*, **2010**, 294, 19-26	5.3	91
219	Ab initio study of hBN nanomeshes on Ru(001), Rh(111), and Pt(111). *Physical Review B*, **2010**, 81,	3.3	55
218	Short-range magnetic order and temperature-dependent properties of cupric oxide. *Journal of Physics Condensed Matter*, **2010**, 22, 045502	1.8	31
217	Cobalt spin states and hyperfine interactions in LaCoO3 investigated by LDA+U calculations. *Physical Review B*, **2010**, 82,	3.3	40
216	Electronic structure of solids with WIEN2k. *Molecular Physics*, **2010**, 108, 3147-3166	1.7	86
215	Iterative diagonalization in augmented plane wave based methods in electronic structure calculations. *Journal of Computational Physics*, **2010**, 229, 453-460	4.1	17
214	Bulk vs. surface effects in ARPES experiment from La2/3Sr1/3MnO3 thin films. *Journal of Electron Spectroscopy and Related Phenomena*, **2010**, 181, 63-69	1.7	7
213	Strong excitonic effects in CuAlO2 delafossite transparent conductive oxides. *Physical Review B*, **2009**, 79,	3.3	68
212	Insight into the performance of GGA functionals for solid-state calculations. *Physical Review B*, **2009** , 80,	3.3	59
211	The small unit cell reconstructions of SrTiO3(111). *Surface Science*, **2009**, 603, 2179-2187	1.8	32
210	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	1.8	18
209	Accurate band gaps of semiconductors and insulators with a semilocal exchange-correlation potential. *Physical Review Letters*, **2009**, 102, 226401	7.4	3253
208	Calculation of the lattice constant of solids with semilocal functionals. *Physical Review B*, **2009**, 79,	3.3	600
207	Density functional calculations on the charge-ordered and valence-mixed modification of YBaFe2O5. *Physical Review B*, **2009**, 79,	3.3	31
206	Bonding of hexagonal BN to transition metal surfaces: An ab initio density-functional theory study. *Physical Review B*, **2008**, 78,	3.3	144
205	Structure and stability of Cd2Nb2O7 and Cd2Ta2O7 explored by ab initio calculations. *Physical Review B*, **2008**, 78,	3.3	36
204	Surface trapping of atoms and molecules with dipole rings. *Science*, **2008**, 319, 1824-6	33.3	147
203	Unraveling the structure of the h-BN/Rh(111) nanomesh with ab initio calculations. *Journal of Physics Condensed Matter*, **2008**, 20, 064207	1.8	38

202	Nuclear quadrupole interaction at S44c in the anatase and rutile modifications of TiO2: Time-differential perturbed-angular-correlation measurements and ab initio calculations. *Physical Review B*, **2008**, 77,	3.3	25
201	PBE+U calculations of the Jahn-Teller effect in PrO2. *Physical Review B*, **2008**, 77,	3.3	32
200	Multiple instabilities in Bi4Ti3O12: A ferroelectric beyond the soft-mode paradigm. *Physical Review B*, **2008**, 77,	3.3	46
199	Effects of three-dimensional band structure in angle- and spin-resolved photoemission from half-metallic La2□Sr1□MnO3. *Physical Review B*, **2008**, 77,	3.3	31
198	Hidden surface states on pristine and H-passivated Ni(111): Angle-resolved photoemission and density-functional calculations. *Physical Review B*, **2008**, 77,	3.3	15
197	Influence of reconstruction on the surface state of Au(110). *Physical Review B*, **2008**, 78,	3.3	31
196	Origin of the light green color and electronic ground state of LaCrO3. *Physical Review B*, **2008**, 77,	3.3	53
195	Force calculation for orbital-dependent potentials with FP-(L)APW + lo basis sets. *Computer Physics Communications*, **2008**, 179, 784-790	4.2	24
194	Ising-type behavior in the antiferromagnetic phase of BaCoO3 from first principles. *Physical Review B*, **2007**, 76,	3.3	8
193	Performance on molecules, surfaces, and solids of the Wu-Cohen GGA exchange-correlation energy functional. *Physical Review B*, **2007**, 75,	3.3	274
192	Single-layer model of the hexagonal boron nitride nanomesh on the Rh(111) surface. *Physical Review Letters*, **2007**, 98, 106802	7.4	135
191	Boron nitride nanomesh: functionality from a corrugated monolayer. *Angewandte Chemie - International Edition*, **2007**, 46, 5115-9	16.4	196
190	Boron Nitride Nanomesh: Functionality from a Corrugated Monolayer. *Angewandte Chemie*, **2007**, 119, 5207-5211	3.6	20
189	The electronic structure and crystal field of RPt3Si (R=Pr, Nd, Sm) compounds. *Physica B: Condensed Matter*, **2007**, 400, 114-118	2.8	5
188	Structural vs electronic origin of renormalized band widths in TTF-TCNQ: An angular dependent NEXAFS study. *Physical Review B*, **2007**, 76,	3.3	11
187	Composite behavior and multidegeneracy in high-pressure phases of Cs and Rb. *Physical Review Letters*, **2007**, 99, 025502	7.4	6
186	Deep multilayer relaxations on the Al(001) surface: Ab initio all-electron calculations. *Physical Review B*, **2007**, 76,	3.3	12
185	Spin-polarized standing waves at an electronically matched interface detected by Fermi-surface photoemission. *Physical Review B*, **2007**, 75,	3.3	6

184	Band gap calculations with Becke□ohnson exchange potential. *Journal of Physics Condensed Matter*, **2007**, 19, 196208	1.8	154
183	Advances in structural analysis of fluoroaluminates using DFT calculations of 27Al electric field gradients. *Journal of Physical Chemistry A*, **2007**, 111, 11873-84	2.8	29
182	Mixed PbFBr1□Ixcrystals: structural and spectroscopic investigations. *Journal of Physics Condensed Matter*, **2007**, 19, 036214	1.8	4
181	Electronic Structure and Optical Properties of AFeO2(A = Ag, Cu) within GGA Calculations. *Chemistry of Materials*, **2007**, 19, 634-640	9.6	81
180	Structure and properties of CoMnSb in the context of half-metallic ferromagnetism. *Physical Review B*, **2006**, 74,	3.3	47
179	Hybrid exchange-correlation energy functionals for strongly correlated electrons: Applications to transition-metal monoxides. *Physical Review B*, **2006**, 74,	3.3	274
178	27Al NMR experiments and quadrupolar parameter ab initio calculations: Crystallographic structure refinement of □Ba3AlF9. *Chemical Physics Letters*, **2006**, 424, 321-326	2.5	20
177	Possible non-collinear magnetic configurations in BaCoO3. *Physica B: Condensed Matter*, **2006**, 378-380, 556-557	2.8	2
176	Electronic quasiparticles and evolution of Fermi level spin states in thin magnetic layers. *Surface Science*, **2006**, 600, 3912-3916	1.8	1
175	The nature of the hydrogen bond in the LaNiSnH2 and NdNiSnH hydrides. *Journal of Chemical Physics*, **2005**, 122, 124703	3.9	2
174	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	2.5	68
173	Magnetic properties of NdNi2B2C from first principles calculations. *Journal of Alloys and Compounds*, **2005**, 403, 29-33	5.7	27
172	Fermi surface and electron correlation effects of ferromagnetic iron. *Physical Review B*, **2005**, 72,	3.3	60
171	Structural investigations of □CaAlF5 by coupling powder XRD, NMR, EPR and spectroscopic parameter calculations. *Journal of Solid State Chemistry*, **2005**, 178, 3655-3661	3.3	23
170	Bandstructure study of magnetic and orbital order in . *Journal of Magnetism and Magnetic Materials* , **2005**, 290-291, 349-352	2.8	2
169	Experimental and theoretical bond critical point properties for model electron density distributions for earth materials. *Physics and Chemistry of Minerals*, **2005**, 32, 114-125	1.6	11
168	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	1.6	52
167	Ab initio electronic structure of rare earth orthoferrites. *Journal of Magnetism and Magnetic Materials*, **2005**, 290-291, 396-399	2.8	15

166	Mössbauer study of LaNiSn and NdNiSn compounds and their deuterides. *Journal of Radioanalytical and Nuclear Chemistry*, **2005**, 266, 553-556	1.5	2
165	Electric field gradients in cuprates: Does LDA+U give the correct charge distribution?. *International Journal of Quantum Chemistry*, **2005**, 101, 550-556	2.1	25
164	Comment on "Taming multiple valency with density functionals: A case study of defective ceria" *Physical Review B*, **2005**, 72,	3.3	81
163	Comparison of empirical bond-valence and first-principles energy calculations for a complex structural instability. *Physical Review B*, **2005**, 72,	3.3	21
162	Momentum selectivity and anisotropy effects in the nitrogen K-edge resonant inelastic x-ray scattering from GaN. *Physical Review B*, **2005**, 72,	3.3	23
161	Geometric frustration, electronic instabilities, and charge singlets in Y2Nb2O7. *Physical Review Letters*, **2004**, 93, 216403	7.4	19
160	Metallic "ferroelectricity" in the pyrochlore Cd2Re2O7. *Physical Review Letters*, **2004**, 92, 065501	7.4	90
159	Magnetic structure and electric-field gradients of uranium dioxide: An ab initio study. *Physical Review B*, **2004**, 69,	3.3	141
158	Competing structural instabilities in the ferroelectric Aurivillius compound SrBi2Ta2O9. *Physical Review B*, **2004**, 70,	3.3	89
157	Band symmetries of GaSe(0001) studied by spin-resolved electron spectroscopy using circularly polarized radiation. *Physical Review B*, **2004**, 69,	3.3	7
156	Competing Instabilities in Ferroelectric Aurivillius Compounds. *Integrated Ferroelectrics*, **2004**, 62, 183-188	0.8	3
155	Band structure effects in nitrogen K-edge resonant inelastic X-ray scattering from GaN. *Physica Status Solidi (B): Basic Research*, **2004**, 241, R27-R29	1.3	10
154	The atomistic origin of the inverse piezoelectric effect in α-quartz. *Journal of Physics and Chemistry of Solids*, **2004**, 65, 1967-1972	3.9	5
153	Evidence for magnetic clusters in BaCoO3. *Physical Review B*, **2004**, 70,	3.3	23
152	Magnetic structure and orbital ordering in BaCoO3 from first-principles calculations. *Physical Review B*, **2004**, 70,	3.3	32
151	Electronic quasiparticle renormalization on the spin wave energy scale. *Physical Review Letters*, **2004**, 92, 097205	7.4	67
150	Structure−Property Relationships in the Nonlinear Optical Crystal KTiOPO4Investigated Using NMR and ab Initio DFT Calculations. *Journal of Physical Chemistry B*, **2004**, 108, 4324-4331	3.4	20
149	Charge-density analysis of YBa2Cu3O6.98. Comparison of theoretical and experimental results. *Acta Crystallographica Section A: Foundations and Advances*, **2003**, 59, 437-51		20

148	Density functional theory investigation of the geometric and spintronic structure of h-BN/Ni(111) in view of photoemission and STM experiments. *Physical Review B*, **2003**, 68,	3.3	165
147	Electronic structure of the quasi-one-dimensional organic conductor TTF-TCNQ. *Physical Review B*, **2003**, 68,	3.3	99
146	Solid state calculations using WIEN2k. *Computational Materials Science*, **2003**, 28, 259-273	3.2	843
145	Charge distribution and chemical bonding in Cu2O. *Physical Review B*, **2003**, 67,	3.3	96
144	Theoretical explanation of the octahedral distortion in FeF2 and MgF2. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2003**, 218,	1	8
143	Electronic structure and transport in type-I and type-VIII clathrates containing strontium, barium, and europium. *Physical Review B*, **2003**, 68,	3.3	239
142	Origin of photoemission final-state effects in Bi2Sr2CaCu2O8 by very-low-energy electron diffraction. *Physical Review B*, **2003**, 68,	3.3	11
141	Comment on "Orthorhombic intermediate state in the zinc blende to rocksalt transformation path of SiC at high pressure". *Physical Review Letters*, **2003**, 90, 049603; author reply 049604	7.4	22
140	Collapse of the antiferromagnetic ground state in the alkali-metal electrosodalites. *Physical Review B*, **2003**, 67,	3.3	5
139	Electronic precursor states of the charge density wave in NbSe3. *Physica B: Condensed Matter*, **2002** , 312-313, 650-652	2.8	
138	Electric field gradients at Ta in Zr and Hf inter-metallic compounds. *Solid State Communications*, **2002**, 121, 525-529	1.6	26
137	Electronic structure calculations of solids using the WIEN2k package for material sciences. *Computer Physics Communications*, **2002**, 147, 71-76	4.2	1260
136	First Principles Calculation of the Crystal Field Splitting in Rare Earth Borocarbides. *European Physical Journal D*, **2002**, 52, 283-286		18
135	On the existence of non-nuclear maxima in simple metals. *Journal of Chemical Physics*, **2002**, 117, 8030-8035	3.3	34
134	Itinerant metamagnetism and possible spin transition in LaCoO3 by temperature/hole doping. *Journal of Applied Physics*, **2002**, 91, 291	2.5	97
133	First-principles study of the ferroelastic phase transition in CaCl2. *Physical Review B*, **2002**, 65,	3.3	14
132	Electronic structure of the pyrochlore metals Cd2Os2O7 and Cd2Re2O7. *Physical Review B*, **2002**, 65,	3.3	73
131	Band- and k-dependent self-energy effects in the unoccupied and occupied quasiparticle band structure of Cu. *Physical Review B*, **2002**, 66,	3.3	20

130	THREE-DIMENSIONAL BAND MAPPING BY COMBINED VERY-LOW-ENERGY ELECTRON DIFFRACTION AND PHOTOEMISSION. *Surface Review and Letters*, **2002**, 09, 1275-1280	1.1	
129	SELF-ENERGY EFFECTS IN THE UNOCCUPIED AND OCCUPIED ELECTRONIC STRUCTURE OF Cu. *Surface Review and Letters*, **2002**, 09, 1281-1285	1.1	1
128	THE FERMI SURFACE IN A MAGNETIC METAL–INSULATOR INTERFACE. *Surface Review and Letters*, **2002**, 09, 1243-1250	1.1	20
127	PEIERLS FLUCTUATIONS IN THE ELECTRON SYSTEM OF A QUASI-ONE-DIMENSIONAL SOLID. *Surface Review and Letters*, **2002**, 09, 1029-1033	1.1	
126	Spectroscopic signatures of spin-charge separation in the quasi-one-dimensional organic conductor TTF-TCNQ. *Physical Review Letters*, **2002**, 88, 096402	7.4	143
125	Defective structure of the ThFe0.2Sn2 and PrFe0.4Sn2 compounds. *Intermetallics*, **2002**, 10, 423-427	3.5	5
124	Electronic structure and electric field gradient calculations of Al2SiO5 polymorphs. *Physics and Chemistry of Minerals*, **2001**, 28, 67-75	1.6	35
123	Electronic structure of the quasi-one-dimensional organic conductor TTF-TCNQ. *Journal of Electron Spectroscopy and Related Phenomena*, **2001**, 114-116, 717-721	1.7	10
122	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		39
121	Electron-density distribution in stishovite, SiO2: a new high-energy synchrotron-radiation study. *Acta Crystallographica Section A: Foundations and Advances*, **2001**, 57, 663-77		44
120	Development and performance analysis of real-world applications for distributed and parallel architectures. *Concurrency Computation Practice and Experience*, **2001**, 13, 841-868	1.4	1
119	Static quadrupole moment of the five-quasiparticle k = 35/2 isomer in (179)w studied with the level-mixing spectroscopy method. *Physical Review Letters*, **2001**, 86, 604-7	7.4	19
118	Spin-orbit splitting of the L-gap surface state on Au(111) and Ag(111). *Physical Review B*, **2001**, 65,	3.3	221
117	Three-dimensional band mapping by angle-dependent very-low-energy electron diffraction and photoemission: Methodology and application to Cu. *Physical Review B*, **2001**, 63,	3.3	37
116	Electronic structure of the sodium and potassium electrosodalites (Na/K)8(AlSiO4)6. *Physical Review B*, **2001**, 64,	3.3	25
115	Correlation induced paramagnetic ground state in FeAl. *Physical Review Letters*, **2001**, 87, 196401	7.4	90
114	High-temperature symmetry breaking in the electronic band structure of the quasi-one-dimensional solid NbSe3. *Physical Review Letters*, **2001**, 87, 196403	7.4	55
113	Efficient linearization of the augmented plane-wave method. *Physical Review B*, **2001**, 64,	3.3	789

112	Electric-field-induced charge-density variations in covalently bonded binary compounds. *Physical Review B*, **2001**, 63,	3.3	20
111	Partial core hole screening in the Cu L 3 edge. *European Physical Journal B*, **2001**, 21, 363-367	1.2	46
110	Electronic structure of fcc Th: Spin-orbit calculation with 6p1/2 local orbital extension. *Physical Review B*, **2001**, 64,	3.3	215
109	A Mössbauer study of the new phases Th4Fe13Sn5 and ThFe0.22Sn2. *Journal of Alloys and Compounds*, **2001**, 317-318, 567-572	5.7	2
108	Electronic structure of the mixed valence system (YM)2BaNiO5 (M=Ca,Sr). *Physical Review B*, **2001**, 63,	3.3	94
107	Electronic Structure Study of CO Adsorption on the Fe(001) Surface. *Journal of Physical Chemistry B*, **2001**, 105, 164-172	3.4	67
106	Investigation of the Negative Thermal Expansion of ZrW2O8. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **2000**, 55, 301-310	1.4	3
105	Improving the efficiency of FP-LAPW calculations. *Computer Physics Communications*, **2000**, 126, 294-309	4.2	181
104	The 3D unoccupied band structure of graphite by very-low-energy electron diffraction. *Applied Surface Science*, **2000**, 162-163, 508-512	6.7	4
103	The orientation-dependent simulation of ELNES. *Ultramicroscopy*, **2000**, 83, 9-16	3.1	67
102	Calculations of electric field gradients in solids: How theory can complement experiment **2000**, 126, 389-395		66
101	Rare earth borocarbides: Electronic structure calculations and electric field gradients. *Physical Review B*, **2000**, 62, 6774-6785	3.3	64
100	Three-dimensional unoccupied band structure of graphite: Very-low-energy electron diffraction and band calculations. *Physical Review B*, **2000**, 61, 4994-5001	3.3	60
99	Electronic structure and optical properties of ThPd3 and UPd3. *Physical Review B*, **2000**, 62, 15547-15552	3.3	5
98	Energy gap of the spin density wave at the Cr(110) surface. *Surface Science*, **2000**, 454-456, 885-890	1.8	8
97	Group V acceptors in CdTe: Ab initio calculation of lattice relaxation and the electric-field gradient. *Physical Review B*, **2000**, 62, R2259-R2262	3.3	45
96	Electronic structure and chemical bonding effects upon the bcc to □phase transition: Ab initio study of Y, Zr, Nb, and Mo. *Physical Review B*, **2000**, 62, 12743-12753	3.3	54
95	Mo cluster formation in the intercalation compound LiMoS2. *Physical Review B*, **2000**, 62, 2397-2400	3.3	77

94	Structure and Properties of NaCl and the Suzuki Phase Na6CdCl8. *Journal of Physical Chemistry B*, **2000**, 104, 1191-1197	3.4	21
93	Study of the static quadrupole moment of theK= 35/2 isomer in. *Journal of Physics G: Nuclear and Particle Physics*, **1999**, 25, 767-769	2.9	5
92	Spin resolved photoemission spectroscopy from InSe(0001) using circularly polarized radiation. *Journal of Physics Condensed Matter*, **1999**, 11, 6715-6723	1.8	2
91	Charge-Density-Wave Mechanism in 2HNbSe2: Photoemission Results. *Physical Review Letters*, **1999**, 82, 4504-4507	7.4	103
90	Electronic structure and heavy-fermion behavior in LiV2O4. *Physical Review B*, **1999**, 60, 16359-16363	3.3	38
89	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	7.4	46
88	Theory of orientation-sensitive near-edge fine-structure core-level spectroscopy. *Physical Review B*, **1999**, 59, 12807-12814	3.3	112
87	Electric field gradient and atomic position for Se in MoSe2 **1999**, 120/121, 423-426		2
86	Accurate Density Functional with Correct Formal Properties: A Step Beyond the Generalized Gradient Approximation. *Physical Review Letters*, **1999**, 82, 2544-2547	7.4	615
85	Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs **1999**, 75, 889-909		519
84	Structure, Chemical Bonding, and Nuclear Quadrupole Interactions of beta-Cd(OH)(2): Experiment and First Principles Calculations. *Inorganic Chemistry*, **1999**, 38, 2860-2867	5.1	20
83	Electronic structure of 1TTiS2. *Physical Review B*, **1999**, 59, 14833-14836	3.3	36
82	Optical properties and band structure of 2HWSe2. *Physical Review B*, **1999**, 60, 8610-8615	3.3	51
81	Electronic structure of 3d-transition-metal oxides: on-site Coulomb repulsion versus covalency. *Journal of Physics Condensed Matter*, **1999**, 11, 1657-1682	1.8	130
80	Evidence for Electron Density Features That Accompany the Noble Gases Solidification. *Journal of Physical Chemistry A*, **1999**, 103, 6209-6213	2.8	7
79	Electronic Structure and Magnetism of Itinerant 5f Ferromagnets URhSi and URhGe **1999**, 487-498		
78	Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs **1999**, 75, 889		15
77	Magnetic order and defect structure of FexAl1 alloys around x=0.5: An experimental and theoretical study. *Physical Review B*, **1998**, 58, 14922-14933	3.3	93

76	Ab initio study of the martensitic bcc-hcp transformation in iron. *Physical Review B*, **1998**, 58, 5296-5304	3.3	105
75	Electric-field-gradient calculations using the projector augmented wave method. *Physical Review B*, **1998**, 57, 14690-14697	3.3	167
74	Absolute Band Mapping by Combined Angle-Dependent Very-Low-Energy Electron Diffraction and Photoemission: Application to Cu. *Physical Review Letters*, **1998**, 81, 4943-4946	7.4	63
73	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	3.3	69
72	Full potential linearized-augmented-plane-wave calculations for 5d transition metals using the relativistic generalized gradient approximation. *Advances in Quantum Chemistry*, **1998**, 33, 209-223	1.4	26
71	Calculation of Electric Field Gradients in Isolated Molecules Using the FPLAPW-Code WIEN95. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **1998**, 53, 411-418	1.4	2
70	Measurement and Calculation of Electric Field Gradients in Hg-Mercaptides. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **1998**, 53, 404-410	1.4	9
69	Occupied and unoccupied electronic band structure of WSe2. *Physical Review B*, **1997**, 55, 10400-10411	3.3	73
68	The theoretical charge density of silicon: experimental testing of exchange and correlation potentials. *Journal of Physics Condensed Matter*, **1997**, 9, 7541-7561	1.8	96
67	LEMS: application of the method to study the static quadrupole moment of the isomer in 179W. *Zeitschrift F Physik A*, **1997**, 358, 267-268		3
66	Electronic Structure Calculations of Hexaborides and Boron Carbide. *Journal of Solid State Chemistry*, **1997**, 133, 51-54	3.3	19
65	Electronic topological transition in zinc metal at high external pressure. *Journal of Physics Condensed Matter*, **1996**, 8, 3581-3599	1.8	20
64	Lattice dynamics and hyperfine interactions in ZnO and ZnSe at high external pressures. *Physical Review B*, **1996**, 53, 11425-11438	3.3	441
63	Electric Field Gradient Calculations of Various Borides. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **1996**, 51, 527-533	1.4	10
62	Calculation of electric hyperfine interaction parameters in solids. *Hyperfine Interactions*, **1996**, 97-98, 1-10	0.8	47
61	(Fe,Mn) Si: Transitions from a magnetic to a nonmagnetic state and from metallic to semiconducting behaviour. *Journal of Magnetism and Magnetic Materials*, **1996**, 157-158, 715-716	2.8	8
60	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	1.8	64
59	Valence-band maximum in the layered semiconductor WSe2: Application of constant-energy contour mapping by photoemission. *Physical Review B*, **1996**, 53, R16152-R16155	3.3	26

58	The fcc - bcc structural transition: II. A mean field model for finite-temperature effects.. *Journal of Physics Condensed Matter*, **1996**, 8, 817-827	1.8	12
57	Ab initio calculation of electric-field-gradient tensors of forsterite. *American Mineralogist*, **1996**, 81, 545-549	2.9	34
56	Description of an LAPW DF Program (WIEN95). *Lecture Notes in Quantum Chemistry II*, **1996**, 139-153	0.6	19
55	Electron spectroscopy on KMnO4. *Journal of Electron Spectroscopy and Related Phenomena*, **1995**, 76, 671-676	1.7	4
54	Electric field gradients, isomer shifts and hyperfine fields from band structure calculations in NiI2. *Hyperfine Interactions*, **1995**, 95, 257-263	0.8	8
53	Magnetism in the Huesler alloys: Co2TiSn and Co2TiAl. *Journal of Magnetism and Magnetic Materials* , **1995**, 140-144, 183-184	2.8	46
52	Band splittings in AF transition metal compounds using the generalized gradient approximation. *Journal of Magnetism and Magnetic Materials*, **1995**, 140-144, 173-174	2.8	1
51	Determination of the nuclear quadrupole moment of 57Fe. *Physical Review Letters*, **1995**, 75, 3545-3548	7.4	235
50	Electronically driven soft modes in zinc metal. *Physical Review Letters*, **1995**, 74, 1139-1142	7.4	60
49	Theoretical investigation of the pressure-induced metallization and the collapse of the antiferromagnetic state of NiI2. *Physical Review B*, **1995**, 51, 4122-4127	3.3	13
48	Electronic structure of PrBa2Cu3O7from LAPW band structure calculations. *Journal of Physics Condensed Matter*, **1994**, 6, 2347-2356	1.8	9
47	Hydrogen Bonding in Potassium Fluoride Dihydrate: A Crystallographic, Spectroscopic, and Theoretical Study. *Inorganic Chemistry*, **1994**, 33, 4774-4780	5.1	8
46	Generalized-gradient-approximation description of band splittings in transition-metal oxides and fluorides. *Physical Review B*, **1994**, 49, 10170-10175	3.3	123
45	Applications of Engel and Vosko's generalized gradient approximation in solids. *Physical Review B*, **1994**, 50, 7279-7283	3.3	321
44	Electronic and magnetic structure of MnF2 and NiF2. *Physical Review B*, **1993**, 48, 12672-12681	3.3	30
43	MAGNETIC PHASES OF BODY CENTERED CUBIC MANGANESE. *International Journal of Modern Physics B*, **1993**, 07, 614-617	1.1	6
42	Structural and electronic properties of InSb under pressure. *Physical Review B*, **1993**, 47, 4841-4848	3.3	22
41	Local susceptibilities in the paramagnetic regime of Y(Fe,Al)2. *Journal of Physics Condensed Matter*, **1993**, 5, 7277-7288	1.8	4

40	Nuclear quadrupole interaction of119mHg in mercury(I) and mercury(II) halides. *Hyperfine Interactions*, **1993**, 80, 1109-1116	0.8	26
39	Electric Field Gradient Calculations of PrBa2Cu3O7. *Springer Series in Solid-state Sciences*, **1993**, 430-433	0.4	
38	Electric-field gradients in YBa2Cu3O7: Discrepancy between experimental and local-density-approximation charge distributions. *Physical Review B*, **1992**, 46, 5849-5852	3.3	32
37	Low-pressure crystalline phases of lithium. *Physical Review B*, **1992**, 45, 5012-5014	3.3	20
36	Electric-field-gradient calculations for systems with large extended-core-state contributions. *Physical Review B*, **1992**, 46, 1321-1325	3.3	92
35	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	1.4	32
34	Isomer shifts and electric field gradients in Y(Fe1−xAlx)2. *Journal of Magnetism and Magnetic Materials*, **1992**, 104-107, 683-684	2.8	5
33	Solid state effects in the molecular crystals of Cl2, Br2 and I2. *Computational and Theoretical Chemistry*, **1992**, 261, 355-365		10
32	Relativistic effects on the structural and magnetic properties of iron. *Solid State Communications*, **1991**, 79, 121-124	1.6	10
31	Electronic structure and electric-field gradients for YBa2Cu4O8 from density-functional calculations. *Physical Review B*, **1991**, 44, 5141-5147	3.3	65
30	Electronic structure and electric field gradients in 2H-TaS2, LiTaS2and SnTaS2. *Journal of Physics Condensed Matter*, **1991**, 3, 9381-9393	1.8	24
29	Calculation of the pressure dependence of the EFG in BCT in, HCP Ti and Zn from energy band structures. *Hyperfine Interactions*, **1990**, 60, 773-776	0.8	7
28	Calculation of EFGs in high Tc superconductors. *Hyperfine Interactions*, **1990**, 61, 1117-1120	0.8	5
27	Full-potential, linearized augmented plane wave programs for crystalline systems. *Computer Physics Communications*, **1990**, 59, 399-415	4.2	2520
26	Charge distribution and electric field gradients in YBa2Cu3O7 by band structure calculations. *International Journal of Quantum Chemistry*, **1990**, 38, 339-347	2.1	5
25	Charge distribution and electric-field gradients in YBa2Cu3O7-x. *Physical Review B*, **1990**, 42, 2051-2061	3.3	236
24	Total Energy Calculations of the Breathing Mode in BaBiO3. *Springer Series in Solid-state Sciences*, **1990**, 343-346	0.4	1
23	Charge Distribution and Electric Field Gradient Calculations for YBa2Cu3O7−x. *Springer Series in Solid-state Sciences*, **1990**, 338-342	0.4	

22	Calculation of the electric field gradient tensor from energy band structures. *Hyperfine Interactions*, **1989**, 51, 917-923	0.8	14
21	Electric-field gradient calculations for YBa2Cu3O7-x. *Journal of Physics Condensed Matter*, **1989**, 1, 4491-4496	1.8	28
20	Electric field gradient in Cu2O from band structure calculations. *Hyperfine Interactions*, **1989**, 52, 153-159	0.8	14
19	Electric field gradient calculations for YBa 2 Cu 3 O 7−δ. *Physica C: Superconductivity and Its Applications*, **1989**, 162-164, 1353-1354	1.3	17
18	First-principles calculation of the electric-field gradient in hcp metals. *Physical Review B*, **1988**, 37, 2792-2796	3.3	259
17	Electronic structure of hcp metals. *Physical Review B*, **1988**, 38, 9368-9374	3.3	87
16	Electron densities in VN. II. Theory. *Physical Review B*, **1987**, 36, 1420-1424	3.3	12
15	A full-potential LAPW study of structural and electronic properties of beryllium. *Journal of Physics F: Metal Physics*, **1987**, 17, 899-911		61
14	Chemical bonding in refractory transition metal compounds with 8, 9, and 10 valence electrons. *Journal of Solid State Chemistry*, **1987**, 70, 199-206	3.3	4
13	Transition metal impurities in copper. *Journal of Magnetism and Magnetic Materials*, **1986**, 54-57, 747-749	2.8	
12	Electronic structure and binding mechanism of Cu2O. *European Physical Journal B*, **1986**, 64, 119-127	1.2	80
11	Electronic structure of chromium and manganese impurities in copper. *Physical Review B*, **1986**, 34, 3572-3576	3.3	15
10	Electronic structure of transition-metal impurities in copper. *Physical Review B*, **1986**, 33, 1706-1716	3.3	31
9	Electron density of TiC. *Journal of Physics F: Metal Physics*, **1985**, 15, 263-266		10
8	Bonding study of TiC and TiN. II. Theory. *Physical Review B*, **1985**, 31, 2316-2325	3.3	84
7	Energy-band-structure studies of NbN(100) and VN(100). *Physical Review B*, **1985**, 32, 575-580	3.3	26
6	Electronic structure and Fermi surface of calcium. *Physical Review B*, **1985**, 32, 7664-7669	3.3	18
5	First-principles calculation of the electric field gradient of Li3N. *Physical Review Letters*, **1985**, 54, 1192-1195	7.4	266

4	Energy-band-structure study of the ZrN(100) surface. *Physical Review B*, **1984**, 30, 635-639	3.3	16
3	Energy bands and electron densities of Li3N. *European Physical Journal B*, **1984**, 57, 273-279	1.2	11
2	Electronic and magnetic structure of BCC Fe-Co alloys from band theory. *Journal of Physics F: Metal Physics*, **1984**, 14, 2659-2671		152
1	Electron densities and chemical bonding in TiC, TiN, and TiO derived from energy band calculations. *International Journal of Quantum Chemistry*, **1983**, 23, 1535-1552	2.1	122