Peter Blaha

List of Publications by Citations

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	Accurate band gaps of semiconductors and insulators with a semilocal exchange-correlation potential. *Physical Review Letters*, **2009**, 102, 226401	7.4	3253
344	Full-potential, linearized augmented plane wave programs for crystalline systems. *Computer Physics Communications*, **1990**, 59, 399-415	4.2	2520
343	Electronic structure calculations of solids using the WIEN2k package for material sciences. *Computer Physics Communications*, **2002**, 147, 71-76	4.2	1260
342	Solid state calculations using WIEN2k. *Computational Materials Science*, **2003**, 28, 259-273	3.2	843
341	Efficient linearization of the augmented plane-wave method. *Physical Review B*, **2001**, 64,	3.3	789
340	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
339	Accurate Density Functional with Correct Formal Properties: A Step Beyond the Generalized Gradient Approximation. *Physical Review Letters*, **1999**, 82, 2544-2547	7.4	615
338	Calculation of the lattice constant of solids with semilocal functionals. *Physical Review B*, **2009**, 79,	3.3	600
337	Merits and limits of the modified Becke-Johnson exchange potential. *Physical Review B*, **2011**, 83,	3.3	584
336	Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs **1999**, 75, 889-909		519
335	Lattice dynamics and hyperfine interactions in ZnO and ZnSe at high external pressures. *Physical Review B*, **1996**, 53, 11425-11438	3.3	441
334	WIEN2k: An APW+lo program for calculating the properties of solids. *Journal of Chemical Physics*, **2020**, 152, 074101	3.9	408
333	Improving the modified Becke-Johnson exchange potential. *Physical Review B*, **2012**, 85,	3.3	383
332	Applications of Engel and Vosko's generalized gradient approximation in solids. *Physical Review B*, **1994**, 50, 7279-7283	3.3	321
331	Performance on molecules, surfaces, and solids of the Wu-Cohen GGA exchange-correlation energy functional. *Physical Review B*, **2007**, 75,	3.3	274
330	Hybrid exchange-correlation energy functionals for strongly correlated electrons: Applications to transition-metal monoxides. *Physical Review B*, **2006**, 74,	3.3	274
329	First-principles calculation of the electric field gradient of Li3N. *Physical Review Letters*, **1985**, 54, 1192-1195	7.4	266

328	First-principles calculation of the electric-field gradient in hcp metals. *Physical Review B*, **1988**, 37, 2792-2796	3.3	259
327	Towards efficient band structure and effective mass calculations for III-V direct band-gap semiconductors. *Physical Review B*, **2010**, 82,	3.3	239
326	Electronic structure and transport in type-I and type-VIII clathrates containing strontium, barium, and europium. *Physical Review B*, **2003**, 68,	3.3	239
325	Charge distribution and electric-field gradients in YBa2Cu3O7-x. *Physical Review B*, **1990**, 42, 2051-2061	3.3	236
324	Determination of the nuclear quadrupole moment of 57Fe. *Physical Review Letters*, **1995**, 75, 3545-3548	7.4	235
323	Spin-orbit splitting of the L-gap surface state on Au(111) and Ag(111). *Physical Review B*, **2001**, 65,	3.3	221
322	Electronic structure of fcc Th: Spin-orbit calculation with 6p1/2 local orbital extension. *Physical Review B*, **2001**, 64,	3.3	215
321	Boron nitride nanomesh: functionality from a corrugated monolayer. *Angewandte Chemie - International Edition*, **2007**, 46, 5115-9	16.4	196
320	Carbon monoxide-induced adatom sintering in a Pd-Fe3O4 model catalyst. *Nature Materials*, **2013**, 12, 724-8	27	191
319	Subsurface cation vacancy stabilization of the magnetite (001) surface. *Science*, **2014**, 346, 1215-8	33.3	181
318	Improving the efficiency of FP-LAPW calculations. *Computer Physics Communications*, **2000**, 126, 294-309	4.2	181
317	Electric-field-gradient calculations using the projector augmented wave method. *Physical Review B*, **1998**, 57, 14690-14697	3.3	167
316	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
315	Band gap calculations with Becke–Johnson exchange potential. *Journal of Physics Condensed Matter*, **2007**, 19, 196208	1.8	154
314	Electronic and magnetic structure of BCC Fe-Co alloys from band theory. *Journal of Physics F: Metal Physics*, **1984**, 14, 2659-2671		152
313	Surface trapping of atoms and molecules with dipole rings. *Science*, **2008**, 319, 1824-6	33.3	147
312	Bonding of hexagonal BN to transition metal surfaces: An ab initio density-functional theory study. *Physical Review B*, **2008**, 78,	3.3	144
311	Spectroscopic signatures of spin-charge separation in the quasi-one-dimensional organic conductor TTF-TCNQ. *Physical Review Letters*, **2002**, 88, 096402	7.4	143

310	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
309	Magnetic structure and electric-field gradients of uranium dioxide: An ab initio study. *Physical Review B*, **2004**, 69,	3.3	141
308	Single-layer model of the hexagonal boron nitride nanomesh on the Rh(111) surface. *Physical Review Letters*, **2007**, 98, 106802	7.4	135
307	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
306	Generalized-gradient-approximation description of band splittings in transition-metal oxides and fluorides. *Physical Review B*, **1994**, 49, 10170-10175	3.3	123
305	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
304	Implementation of screened hybrid functionals based on the Yukawa potential within the LAPW basis set. *Physical Review B*, **2011**, 83,	3.3	121
303	Spin-state crossover and hyperfine interactions of ferric iron in MgSiO(3) perovskite. *Physical Review Letters*, **2011**, 106, 118501	7.4	121
302	Theory of orientation-sensitive near-edge fine-structure core-level spectroscopy. *Physical Review B*, **1999**, 59, 12807-12814	3.3	112
301	Ab initio study of the martensitic bcc-hcp transformation in iron. *Physical Review B*, **1998**, 58, 5296-5304	3.3	105
300	Understanding the L2,3 x-ray absorption spectra of early 3d transition elements. *Physical Review B*, **2010**, 82,	3.3	103
299	Charge-Density-Wave Mechanism in 2H□NbSe2: Photoemission Results. *Physical Review Letters*, **1999**, 82, 4504-4507	7.4	103
298	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
297	Electronic structure of the quasi-one-dimensional organic conductor TTF-TCNQ. *Physical Review B*, **2003**, 68,	3.3	99
296	Itinerant metamagnetism and possible spin transition in LaCoO3 by temperature/hole doping. *Journal of Applied Physics*, **2002**, 91, 291	2.5	97
295	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
294	Charge distribution and chemical bonding in Cu2O. *Physical Review B*, **2003**, 67,	3.3	96
293	Electronic structure of the mixed valence system (YM)2BaNiO5 (M=Ca,Sr). *Physical Review B*, **2001**, 63,	3.3	94

292	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
291	Oxide heterostructures for efficient solar cells. *Physical Review Letters*, **2013**, 110, 078701	7.4	92
290	Electric-field-gradient calculations for systems with large extended-core-state contributions. *Physical Review B*, **1992**, 46, 1321-1325	3.3	92
289	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
288	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
287	Metallic "ferroelectricity" in the pyrochlore Cd2Re2O7. *Physical Review Letters*, **2004**, 92, 065501	7.4	90
286	Correlation induced paramagnetic ground state in FeAl. *Physical Review Letters*, **2001**, 87, 196401	7.4	90
285	Competing structural instabilities in the ferroelectric Aurivillius compound SrBi2Ta2O9. *Physical Review B*, **2004**, 70,	3.3	89
284	Electronic structure of hcp metals. *Physical Review B*, **1988**, 38, 9368-9374	3.3	87
283	Electronic structure of solids with WIEN2k. *Molecular Physics*, **2010**, 108, 3147-3166	1.7	86
282	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
281	Bonding study of TiC and TiN. II. Theory. *Physical Review B*, **1985**, 31, 2316-2325	3.3	84
280	Electronic Structure and Optical Properties of AFeO2(A = Ag, Cu) within GGA Calculations. *Chemistry of Materials*, **2007**, 19, 634-640	9.6	81
279	Comment on aming multiple valency with density functionals: A case study of defective ceria *Physical Review B*, **2005**, 72,	3.3	81
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277	Electronic structure and binding mechanism of Cu2O. *European Physical Journal B*, **1986**, 64, 119-127	1.2	80
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273	Construction of an optimal GGA functional for molecules and solids. *Physical Review B*, **2011**, 83,	3.3	71
272	Epitaxial growth of hexagonal boron nitride on Ag(111). *Physical Review B*, **2010**, 82,	3.3	69
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269	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
268	Electronic quasiparticle renormalization on the spin wave energy scale. *Physical Review Letters*, **2004**, 92, 097205	7.4	67
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265	Calculations of electric field gradients in solids: How theory can complement experiment **2000**, 126, 389-395		66
264	Electronic structure and electric-field gradients for YBa2Cu4O8 from density-functional calculations. *Physical Review B*, **1991**, 44, 5141-5147	3.3	65
263	Rare earth borocarbides: Electronic structure calculations and electric field gradients. *Physical Review B*, **2000**, 62, 6774-6785	3.3	64
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261	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
260	Room-temperature spin-spiral multiferroicity in high-pressure cupric oxide. *Nature Communications*, **2013**, 4, 2511	17.4	61
259	Adsorption and incorporation of transition metals at the magnetite Fe3O4(001) surface. *Physical Review B*, **2015**, 92,	3.3	61
258	Ferromagnetic insulating state in tensile-strained LaCoO3 thin films from LDA + U calculations. *Physical Review B*, **2012**, 85,	3.3	61
257	A full-potential LAPW study of structural and electronic properties of beryllium. *Journal of Physics F: Metal Physics*, **1987**, 17, 899-911		61

256	Fermi surface and electron correlation effects of ferromagnetic iron. *Physical Review B*, **2005**, 72,	3.3	60
255	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
254	Electronically driven soft modes in zinc metal. *Physical Review Letters*, **1995**, 74, 1139-1142	7.4	60
253	Insight into the performance of GGA functionals for solid-state calculations. *Physical Review B*, **2009**, 80,	3.3	59
252	Atomic-Scale Structure of the Hematite □FeO(11 02) "R-Cut" Surface. *Journal of Physical Chemistry C*, **2018**, 122, 1657-1669	3.8	59
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244	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
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228	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
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223	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
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210	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
209	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
208	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
207	Calculating NMR chemical shifts using the augmented plane-wave method. *Physical Review B*, **2014**, 89,	3.3	31
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205	Short-range magnetic order and temperature-dependent properties of cupric oxide. *Journal of Physics Condensed Matter*, **2010**, 22, 045502	1.8	31
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173	Evidence for magnetic clusters in BaCoO3. *Physical Review B*, **2004**, 70,	3.3	23
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171	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
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