Peter Blchl

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

103 papers	64,290 citations	44 h-index	108 g-index
108 ext. papers	73,161 ext. citations	5.6 avg, IF	8.58 L-index

#	Paper	IF	Citations
103	Orbital-order phase transition in Pr1−xCaxMnO3 probed by photovoltaics. *Physical Review B*, **2021**, 103,	3.3	2
102	Ultrafast spin-nematic and ferroelectric phase transitions induced by femtosecond light pulses. *Physical Review B*, **2020**, 102,	3.3	1
101	Hybrid density functional theory benchmark study on lithium manganese oxides. *Physical Review B*, **2020**, 101,	3.3	10
100	Evolution of the magnetic and polaronic order of Pr1/2Ca1/2MnO3 following an ultrashort light pulse. *Physical Review B*, **2020**, 102,	3.3	3
99	Dynamic observation of manganese adatom mobility at perovskite oxide catalyst interfaces with water. *Communications Materials*, **2020**, 1,	6	9
98	A Review of Density Functional Models for the Description of Fe(II) Spin-Crossover Complexes. *Molecules*, **2020**, 25,	4.8	6
97	Closing the gap between theory and experiment for lithium manganese oxide spinels using a high-dimensional neural network potential. *Physical Review B*, **2020**, 102,	3.3	10
96	Predicting oxidation and spin states by high-dimensional neural networks: Applications to lithium manganese oxide spinels. *Journal of Chemical Physics*, **2020**, 153, 164107	3.9	11
95	Surface resonance of the (2□) reconstructed lanthanum hexaboride (001)-cleavage plane: A combined STM and DFT study. *Physical Review B*, **2019**, 100,	3.3	3
94	Adaptive cluster approximation for reduced density-matrix functional theory. *Physical Review B*, **2018**, 97,	3.3	1
93	Density functional study of half-metallicity and spin polarization in Fe T S with T = Mn,Ni. *Journal of Physics Condensed Matter*, **2018**, 30, 305501	1.8	3
92	Relaxation of photoexcitations in polaron-induced magnetic microstructures. *Physical Review B*, **2018**, 97,	3.3	3
91	Evolution of Hot Polaron States with a Nanosecond Lifetime in a Manganite Perovskite. *Advanced Energy Materials*, **2017**, 7, 1602174	21.8	16
90	Reduced density-matrix functionals from many-particle theory. *European Physical Journal: Special Topics*, **2017**, 226, 2677-2692	2.3	16
89	Electronic structure of Pr1−xCaxMnO3. *Physical Review B*, **2017**, 95,	3.3	23
88	Reduced density-matrix functionals applied to the Hubbard dimer. *Physical Review B*, **2016**, 93,	3.3	16
87	Beam matching: A method to study phonon transport through interfaces and multilayer structures. *Physica Status Solidi (A) Applications and Materials Science*, **2016**, 213, 635-648	1.6	1

86	Temperature- and doping-dependent optical absorption in the small-polaron system Pr1−xCaxMnO3. *Physical Review B*, **2015**, 92,	3.3	23
85	Density-matrix functionals from Green's functions. *Physical Review B*, **2013**, 88,	3.3	27
84	In Situ Electrochemical Electron Microscopy Study of Oxygen Evolution Activity of Doped Manganite Perovskites. *Advanced Functional Materials*, **2012**, 22, 3378-3388	15.6	63
83	Method to include explicit correlations into density-functional calculations based on density-matrix functional theory. *Physical Review B*, **2011**, 84,	3.3	15
82	Theoretical study of interaction of laser with diatomic molecules using the Basis Generator Method. *Journal of Physics: Conference Series*, **2009**, 194, 032052	0.3	
81	Dynamical dimer method for the determination of transition states with ab initio molecular dynamics. *Journal of Chemical Physics*, **2008**, 128, 044107	3.9	8
80	Ammonia production at the FeMo cofactor of nitrogenase: results from density functional theory. *Journal of the American Chemical Society*, **2007**, 129, 2998-3006	16.4	104
79	Modeling of Growth of High-κ Oxides on Semiconductors **2007**, 165-179		
78	Band alignment at the La2Hf2O7(001)Si interface. *Applied Physics Letters*, **2006**, 88, 202903	3.4	28
77	Molecular design of interfaces based on density-functional simulations. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2006**, 632, 2075-2075	1.3	
76	Model for acetylene reduction by nitrogenase derived from density functional theory. *Inorganic Chemistry*, **2005**, 44, 4568-75	5.1	29
75	Electronic Structure Methods: Augmented Waves, Pseudopotentials and The Projector Augmented Wave Method **2005**, 93-119		11
74	Towards an understanding of the workings of nitrogenase from DFT calculations. *ChemPhysChem*, **2005**, 6, 1724-6	3.2	36
73	Ab-initio simulations on growth and interface properties of epitaxial oxides on silicon. *Microelectronic Engineering*, **2005**, 80, 402-407	2.5	5
72	Structural and electronic properties of the interface between the high-k Oxide LaAlO3 and Si(001). *Physical Review Letters*, **2005**, 95, 137602	7.4	52
71	Activation and protonation of dinitrogen at the FeMo cofactor of nitrogenase. *Journal of Chemical Physics*, **2005**, 123, 074306	3.9	39
70	First-principles calculations of strontium on Si(001). *Physical Review B*, **2004**, 69,	3.3	58
69	Chemistry of La on the Si(001) surface from first principles. *Physical Review B*, **2004**, 70,	3.3	16

68	The interface between silicon and a high-k oxide. *Nature*, **2004**, 427, 53-6	50.4	266
67	Interaction of NaCl with solid water. *Journal of Chemical Physics*, **2004**, 121, 9671-8	3.9	19
66	Projector augmented wave method:ab initio molecular dynamics with full wave functions. *Bulletin of Materials Science*, **2003**, 26, 33-41	1.7	274
65	Implementation of an all-electron GW approximation based on the projector augmented wave method without plasmon pole approximation: Application to Si, SiC, AlAs, InAs, NaH, and KH. *Physical Review B*, **2003**, 67,	3.3	176
64	Heteroepitaxial growth of high-k gate oxides on silicon: insights from first-principles calculations on Zr on Si(0 0 1). *Computational Materials Science*, **2003**, 27, 70-74	3.2	12
63	Nitrogen binding to the FeMo-cofactor of nitrogenase. *Journal of the American Chemical Society*, **2003**, 125, 15772-8	16.4	102
62	Ab initio molecular dynamics with a continuum solvation model. *Journal of Chemical Physics*, **2003**, 118, 1089-1100	3.9	31
61	Sampling Phase Space by a Combined QM/MM ab Initio Car□Parrinello Molecular Dynamics Method with Different (Multiple) Time Steps in the Quantum Mechanical (QM) and Molecular Mechanical (MM) Domains. *Journal of Physical Chemistry A*, **2002**, 106, 1173-1182	2.8	13
60	A Car□Parrinello study of the formation of oxidizing intermediates from Fenton's reagent in aqueous solution. *Physical Chemistry Chemical Physics*, **2002**, 4, 3619-3627	3.6	79
59	Second-generation wave-function thermostat for ab initio molecular dynamics. *Physical Review B*, **2002**, 65,	3.3	16
58	LDA+U calculated electronic and structural properties of NiO(001) and NiO(111) p(2□) surfaces. *Computational Materials Science*, **2002**, 24, 192-198	3.2	27
57	Chemical Involvement of Solvent Water Molecules in Elementary Steps of the Fenton Oxidation Reaction. *Angewandte Chemie*, **2001**, 113, 2977-2979	3.6	7
56	Chemical Involvement of Solvent Water Molecules in Elementary Steps of the Fenton Oxidation Reaction. *Angewandte Chemie - International Edition*, **2001**, 40, 2893-2895	16.4	71
55	Solvation Effects on the SN2 Reaction between CH3Cl and Cl- in Water. *Journal of Physical Chemistry A*, **2001**, 105, 3300-3310	2.8	79
54	Chemical Involvement of Solvent Water Molecules in Elementary Steps of the Fenton Oxidation Reaction We gratefully acknowledge the helpful discussions with Michiel Gribnau (Unilever-Vlaardingen) and we thank the Netherlands Organization for Scientific Research (NWO) for support through the PPM-CMS program and the NCF for providing computer time.. *Angewandte*	16.4	4
53	Phosphane lone-pair energies as a measure of ligand donor strengths and relation to activation energies. *Computational and Theoretical Chemistry*, **2000**, 506, 233-242		19
52	Towards solvation simulations with a combined ab initio molecular dynamics and molecular mechanics approach. *Computational and Theoretical Chemistry*, **2000**, 506, 313-334		20
51	Taming the ground-state and optical properties of transition metal oxides. *Computational Materials Science*, **2000**, 17, 146-150	3.2	2

50	Implementation of the projector augmented-wave LDA+U method: Application to the electronic structure of NiO. *Physical Review B*, **2000**, 62, 16392-16401	3.3	436
49	First-principles calculations of defects in oxygen-deficient silica exposed to hydrogen. *Physical Review B*, **2000**, 62, 6158-6179	3.3	299
48	Toward an Alkene Hydroamination Catalyst: Static and Dynamic ab Initio DFT Studies. *Journal of the American Chemical Society*, **2000**, 122, 4098-4107	16.4	152
47	Monomer Capture in Brookhart's Ni(II) Diimine Olefin Polymerization Catalyst: Static and Dynamic Quantum Mechanics/Molecular Mechanics Study. *Journal of Physical Chemistry A*, **2000**, 104, 121-129	2.8	65
46	Hydrogen Electrochemistry and Stress-Induced Leakage Current in Silica. *Physical Review Letters*, **1999**, 83, 372-375	7.4	265
45	First-principles molecular dynamics study of small molecules in zeolites. *Catalysis Today*, **1999**, 50, 501-509	3.3	27
44	Aspects of defects in silica related to dielectric breakdown of gate oxides in MOSFETs. *Physica B: Condensed Matter*, **1999**, 273-274, 1022-1026	2.8	33
43	Molecular Reaction Modeling from Ab-Initio Molecular Dynamics. *ACS Symposium Series*, **1999**, 88-99	0.4	5
42	First principles investigations of a quasi-one-dimensional charge-transfer molecular crystal: TTF-2,5Cl2BQ. *Computational Materials Science*, **1998**, 10, 325-329	3.2	5
41	Evidence for a Stable Ti(IV) Metallocene Dihydrogen Complex from ab Initio Molecular Dynamics. *Journal of the American Chemical Society*, **1998**, 120, 2174-2175	16.4	47
40	Electric-field-gradient calculations using the projector augmented wave method. *Physical Review B*, **1998**, 57, 14690-14697	3.3	167
39	Ab initio calculation of binding and diffusion of a Ga adatom on the GaAs (001)-(4×4) surface. *Physical Review B*, **1998**, 58, 1499-1505	3.3	33
38	Static and ab Initio Molecular Dynamics Study of the Titanium(IV)-Constrained Geometry Catalyst (CpSiH2NH)Ti-R+. 2. Chain Termination and Long Chain Branching. *Organometallics*, **1997**, 16, 3454-3468	3.8	111
37	A Combined Car-Parrinello QM/MM Implementation for ab Initio Molecular Dynamics Simulations of Extended Systems: Application to Transition Metal Catalysis. *Journal of Physical Chemistry B*, **1997**, 101, 7877-7880	3.4	87
36	Hydrocarbon adsorption on Si(001): when does the Si dimer bond break?. *Surface Science*, **1997**, 374, 298-305	1.8	94
35	Ab-initio calculations of one-dimensional band structures of mixed-stack molecular crystals. *Solid State Communications*, **1997**, 102, 589-594	1.6	19
34	Ab initio molecular dynamics calculations to study catalysis. *International Journal of Quantum Chemistry*, **1997**, 61, 369-380	2.1	29
33	Ab Initio Molecular Dynamics with the Projector Augmented Wave Method. *ACS Symposium Series*, **1996**, 54-69	0.4	9

32	A Dynamical Density Functional Study on the Reaction of Ethylene with Cp2Zr(C2H5)+. *Journal of the American Chemical Society*, **1996**, 118, 4434-4441	16.4	117
31	Migratory CO Insertion and Aldehyde Formation in Carbonylation of Methane by the Rh(PH3)2Cl Catalyst. A Dynamical Density Functional Study. *Journal of the American Chemical Society*, **1996**, 118, 5412-5419	16.4	40
30	Combined Static and Dynamic Density Functional Study of the Ti(IV) Constrained Geometry Catalyst (CpSiH2NH)TiR+. 1. Resting States and Chain Propagation. *Journal of the American Chemical Society*, **1996**, 118, 13021-13030	16.4	144
29	First-Principles Investigation of Enantioselective Catalysis: Asymmetric Allylic Amination with Pd Complexes Bearing P,N-Ligands. *Organometallics*, **1996**, 15, 4125-4132	3.8	118
28	Struktur und Dynamik von Methanol in einem Zeolithen. *Angewandte Chemie*, **1996**, 108, 187-189	3.6	17
27	Interaction of water and methanol with a zeolite at high coverages. *Chemical Physics Letters*, **1996**, 253, 448-455	2.5	77
26	Structure and Dynamics of Methanol in a Zeolite. *Angewandte Chemie International Edition in English*, **1996**, 35, 175-177		75
25	Ab initio molecular-dynamics study of diffusion and defects in solid Li3N. *Physical Review B*, **1996**, 53, 9084-9091	3.3	48
24	First-principles molecular-dynamics simulations for neutral p-chloranil and its radical anion. *Physical Review B*, **1996**, 53, 12112-12120	3.3	33
23	Electronic structure of the Cu, Zn superoxide dismutase active site and its interactions with the substrate. *The Journal of Physical Chemistry*, **1995**, 99, 1338-1348		60
22	Dynamics of beryllocene. *Journal of Chemical Physics*, **1995**, 103, 683-690	3.9	33
21	Reaction of Methane with Rh(PH3)2Cl: A Dynamical Density Functional Study. *Journal of the American Chemical Society*, **1995**, 117, 12625-12634	16.4	55
20	Electrostatic decoupling of periodic images of plane-wave-expanded densities and derived atomic point charges. *Journal of Chemical Physics*, **1995**, 103, 7422-7428	3.9	190
19	Finite-temperature characterization of ferrocene from first-principles molecular dynamics simulations. *Journal of Chemical Physics*, **1994**, 100, 8194-8203	3.9	44
18	Projector augmented-wave method. *Physical Review B*, **1994**, 50, 17953-17979	3.3	50591
17	Improved tetrahedron method for Brillouin-zone integrations. *Physical Review B*, **1994**, 49, 16223-16233	3.3	5100
16	Fluxional Dynamics of Beryllocene. *Journal of the American Chemical Society*, **1994**, 116, 11177-11178	16.4	35
15	First-principles calculations of self-diffusion constants in silicon. *Physical Review Letters*, **1993**, 70, 2435-2438	7.4	240

14	Adsorption and scanning-tunneling-microscope imaging of benzene on graphite and MoS2. *Physical Review Letters*, **1993**, 70, 3263-3266	7.4	126
13	First-principles calculations of hyperfine parameters. *Physical Review B*, **1993**, 47, 4244-4255	3.3	208
12	Hypothetical Carbon Modifications Derived from Zeolite Frameworks. *Angewandte Chemie International Edition in English*, **1993**, 32, 701-703		58
11	Crystal orbital Hamilton populations (COHP): energy-resolved visualization of chemical bonding in solids based on density-functional calculations. *The Journal of Physical Chemistry*, **1993**, 97, 8617-8624		2018
10	Native defects and self-compensation in ZnSe. *Physical Review B*, **1992**, 45, 10965-10978	3.3	253
9	Interacting loop-current model of superconducting networks. *Journal of Low Temperature Physics*, **1992**, 88, 163-195	1.3	16
8	Adiabaticity in first-principles molecular dynamics. *Physical Review B*, **1992**, 45, 9413-9416	3.3	279
7	Electronic structure of ordered and disordered Pd3Fe. *Journal of Magnetism and Magnetic Materials* , **1990**, 87, 97-105	2.8	15
6	First-principles calculations of diffusion coefficients: Hydrogen in silicon. *Physical Review Letters*, **1990**, 64, 1401-1404	7.4	78
5	Phase boundary of superconducting networks: A new approximation scheme. *Physical Review B*, **1990**, 42, 76-79	3.3	7
4	Das et al. reply. *Physical Review Letters*, **1990**, 65, 2084	7.4	3
3	Generalized separable potentials for electronic-structure calculations. *Physical Review B*, **1990**, 41, 5414-5416	3.3	236
2	Electronic structure and Schottky-barrier heights of (111) NiSi2/Si A- and B-type interfaces. *Physical Review Letters*, **1989**, 63, 1168-1171	7.4	125
1	Electronic structure and properties of NiSi2 and CoSi2 in the fluorite and adamantane structures. *Physical Review B*, **1987**, 36, 2493-2503	3.3	103