Peter BlÃ¶chl

List of Publications by Year in descending order

106 papers	82,440 citations	50170 46 h-index	31759 101 g-index
108 all docs	108 docs citations	108 times ranked	54759 citing authors

#	Article	IF	Citations
1	Real-time non-adiabatic dynamics in the one-dimensional Holstein model: Trajectory-based vs exact methods. Journal of Chemical Physics, 2022, 156, .	1.2	6
2	Orbital-order phase transition in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Pr</mml:mi><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi>Mn</mml:mi><mml:mn>1</mml:mn></mml:msub></mml:mrow></mml:math> probed by photovoltaics. Physical Review B, 2021, 103, .	1.1	5
3	Hydrogen-related defects in titanium dioxide at the interface to palladium. Physical Review Materials, 2021, 5, .	0.9	1
4	Dynamic observation of manganese adatom mobility at perovskite oxide catalyst interfaces with water. Communications Materials, 2020, 1, .	2.9	19
5	A Review of Density Functional Models for the Description of Fe(II) Spin-Crossover Complexes. Molecules, 2020, 25, 5176.	1.7	8
6	Closing the gap between theory and experiment for lithium manganese oxide spinels using a high-dimensional neural network potential. Physical Review B, 2020, 102, .	1.1	24
7	Predicting oxidation and spin states by high-dimensional neural networks: Applications to lithium manganese oxide spinels. Journal of Chemical Physics, 2020, 153, 164107.	1.2	26
8	Ultrafast spin-nematic and ferroelectric phase transitions induced by femtosecond light pulses. Physical Review B, 2020, 102, .	1.1	5
9	Hybrid density functional theory benchmark study on lithium manganese oxides. Physical Review B, 2020, 101, .	1.1	12
10	Evolution of the magnetic and polaronic order of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Pr</mml:mi><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi>Mn</mml:mi><mml:mn>1</mml:mn></mml:msub></mml:mrow></mml:math> following an ultrashort light pulse. Physical Review B, 2020, 102, .	1.1	8
11	Surface resonance of the (2Ã—1) reconstructed lanthanum hexaboride (001)-cleavage plane: A combined STM and DFT study. Physical Review B, 2019, 100, .	1.1	4
12	Adaptive cluster approximation for reduced density-matrix functional theory. Physical Review B, 2018, 97, .	1.1	5
13	Density functional study of half-metallicity and spin polarization in Fe_{1â^'x}T_xS₂ with Tâ€‰â€‰=â€‰â€‰Mn,Ni. Journal of Physics Condensed Matter, 2018, 30, 305501.	0.7	3
14	Relaxation of photoexcitations in polaron-induced magnetic microstructures. Physical Review B, 2018, 97, .	1.1	6
15	Evolution of Hot Polaron States with a Nanosecond Lifetime in a Manganite Perovskite. Advanced Energy Materials, 2017, 7, 1602174.	10.2	24
16	Reduced density-matrix functionals from many-particle theory. European Physical Journal: Special Topics, 2017, 226, 2677-2692.	1.2	26
17	Electronic structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Pr</mml:mi><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi>Mn</mml:mi><mml:mn>1</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2017, 95, .	1.1	34
18	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.	0.8	1

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19	Reduced density-matrix functionals applied to the Hubbard dimer. Physical Review B, 2016, 93, .	1.1	20
20	Publisher's Note: Temperature- and doping-dependent optical absorption in the small-polaron system <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Pr</mml:mi><mml:mrow><mml:mn>1</mml:mn> [Phys. Rev. B 92, 035145 (2015)]. Physical Review B, 2016, 94, .	1.1	0
21	Publisher's Note: Temperature- and doping-dependent optical absorption in the small-polaron system <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">P</mml:mi><mml:msub><mml:mi mathvariant="normal">r</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">a</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi>Mn</mml:mi><mml:mi	1.1	29
22	Resolvent approach for the evaluation of the reduced density-matrix functional of correlated electron systems. , 2013, , .		0
23	Density-matrix functionals from Green's functions. Physical Review B, 2013, 88, .	1.1	27
24	In Situ Electrochemical Electron Microscopy Study of Oxygen Evolution Activity of Doped Manganite Perovskites. Advanced Functional Materials, 2012, 22, 3378-3388.	7.8	79
25	Method to include explicit correlations into density-functional calculations based on density-matrix functional theory. Physical Review B, 2011, 84, .	1.1	16
26	Theoretical study of interaction of laser with diatomic molecules using the Basis Generator Method. Journal of Physics: Conference Series, 2009, 194, 032052.	0.3	0
27	Dynamical dimer method for the determination of transition states with ab initio molecular dynamics. Journal of Chemical Physics, 2008, 128, 044107.	1.2	9
28	Ammonia Production at the FeMo Cofactor of Nitrogenase:â€‰ Results from Density Functional Theory. Journal of the American Chemical Society, 2007, 129, 2998-3006.	6.6	125
29	Modeling of Growth of High-Î² Oxides on Semiconductors. , 2007, , 165-179.		0
30	Molecular design of interfaces based on density-functional simulations. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2006, 632, 2075-2075.	0.6	0
31	Band alignment at the La2Hf2O7â^•(001)Si interface. Applied Physics Letters, 2006, 88, 202903.	1.5	31
32	Towards an Understanding of the Workings of Nitrogenase from DFT Calculations. ChemPhysChem, 2005, 6, 1724-1726.	1.0	45
33	Ab-initio simulations on growth and interface properties of epitaxial oxides on silicon. Microelectronic Engineering, 2005, 80, 402-407.	1.1	5
34	Structural and Electronic Properties of the Interface between the High-kOxideLaAlO3and Si(001). Physical Review Letters, 2005, 95, 137602.	2.9	54
35	Activation and protonation of dinitrogen at the FeMo cofactor of nitrogenase. Journal of Chemical Physics, 2005, 123, 074306.	1.2	49
36	Model for Acetylene Reduction by Nitrogenase Derived from Density Functional Theory. Inorganic Chemistry, 2005, 44, 4568-4575.	1.9	32

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37	Electronic Structure Methods: Augmented Waves, Pseudopotentials and The Projector Augmented Wave Method. , 2005, , 93-119.		20
38	First-principles calculations of strontium on Si(001). Physical Review B, 2004, 69, .	1.1	62
39	Chemistry of La on the Si(001) surface from first principles. Physical Review B, 2004, 70, .	1.1	16
40	The interface between silicon and a high-k oxide. Nature, 2004, 427, 53-56.	13.7	280
41	Interaction of NaCl with solid water. Journal of Chemical Physics, 2004, 121, 9671-9678.	1.2	19
42	Projector augmented wave method:ab initio molecular dynamics with full wave functions. Bulletin of Materials Science, 2003, 26, 33-41.	0.8	374
43	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, .	1.1	199
44	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.	1.4	13
45	Nitrogen Binding to the FeMo-Cofactor of Nitrogenase. Journal of the American Chemical Society, 2003, 125, 15772-15778.	6.6	109
46	Ab initio molecular dynamics with a continuum solvation model. Journal of Chemical Physics, 2003, 118, 1089-1100.	1.2	38
47	Sampling Phase Space by a Combined QM/MM ab Initio Carâ˜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.	1.1	16
48	A Carâ€“Parrinello study of the formation of oxidizing intermediates from Fenton's reagent in aqueous solution. Physical Chemistry Chemical Physics, 2002, 4, 3619-3627.	1.3	84
49	Second-generation wave-function thermostat forab initiomolecular dynamics. Physical Review B, 2002, 65, .	1.1	18
50	LDA+U calculated electronic and structural properties of NiO(001) and NiO(111) p(2Ã—2) surfaces. Computational Materials Science, 2002, 24, 192-198.	1.4	29
51	Solvation Effects on the SN2 Reaction between CH3Cl and Cl-in Water. Journal of Physical Chemistry A, 2001, 105, 3300-3310.	1.1	87
52	Chemical Involvement of Solvent Water Molecules in Elementary Steps of the Fenton Oxidation Reaction. Angewandte Chemie - International Edition, 2001, 40, 2893-2895.	7.2	79
53	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 Chemie - International Edition, 2001, 40, 2893-2895.	7.2	4
54	Phosphane lone-pair energies as a measure of ligand donor strengths and relation to activation energies. Computational and Theoretical Chemistry, 2000, 506, 233-242.	1.5	22

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55	Towards solvation simulations with a combined ab initio molecular dynamics and molecular mechanics approach. Computational and Theoretical Chemistry, 2000, 506, 313-334.	1.5	22
56	Taming the ground-state and optical properties of transition metal oxides. Computational Materials Science, 2000, 17, 146-150.	1.4	2
57	Implementation of the projector augmented-wave LDA+U method: Application to the electronic structure of NiO. Physical Review B, 2000, 62, 16392-16401.	1.1	494
58	First-principles calculations of defects in oxygen-deficient silica exposed to hydrogen. Physical Review B, 2000, 62, 6158-6179.	1.1	346
59	Toward an Alkene Hydroamination Catalyst:â€‰ Static and Dynamic ab Initio DFT Studies. Journal of the American Chemical Society, 2000, 122, 4098-4107.	6.6	166
60	Monomer Capture in Brookhart's Ni(II) Diimine Olefin Polymerization Catalyst:Â Static and Dynamic Quantum Mechanics/Molecular Mechanics Study. Journal of Physical Chemistry A, 2000, 104, 121-129.	1.1	73
61	Hydrogen Electrochemistry and Stress-Induced Leakage Current in Silica. Physical Review Letters, 1999, 83, 372-375.	2.9	312
62	First-principles molecular dynamics study of small molecules in zeolites. Catalysis Today, 1999, 50, 501-509.	2.2	30
63	Aspects of defects in silica related to dielectric breakdown of gate oxides in MOSFETs. Physica B: Condensed Matter, 1999, 273-274, 1022-1026.	1.3	37
64	Molecular Reaction Modeling from Ab-Initio Molecular Dynamics. ACS Symposium Series, 1999, , 88-99.	0.5	8
65	First principles investigations of a â€œquasi-one-dimensionalâ€•charge-transfer molecular crystal: TTF-2,5Cl2BQ. Computational Materials Science, 1998, 10, 325-329.	1.4	5
66	Evidence for a Stable Ti(IV) Metallocene Dihydrogen Complex from ab Initio Molecular Dynamics. Journal of the American Chemical Society, 1998, 120, 2174-2175.	6.6	50
67	Electric-field-gradient calculations using the projector augmented wave method. Physical Review B, 1998, 57, 14690-14697.	1.1	187
68	Ab initiocalculation of binding and diffusion of a Ga adatom on theGaAsâ€‚(001)â˜c(4Ã—4)surface. Physical Review B, 1998, 58, 1499-1505.	1.1	33
69	Static andab InitioMolecular Dynamics Study of the Titanium(IV)-Constrained Geometry Catalyst (CpSiH2NH)Ti-R+. 2. Chain Termination and Long Chain Branching. Organometallics, 1997, 16, 3454-3468.	1.1	120
70	A Combined Carâ˜Parrinello QM/MM Implementation for ab Initio Molecular Dynamics Simulations of Extended Systems:Â Application to Transition Metal Catalysis. Journal of Physical Chemistry B, 1997, 101, 7877-7880.	1.2	121
71	Hydrocarbon adsorption on Si(001): when does the Si dimer bond break?. Surface Science, 1997, 374, 298-305.	0.8	97
72	Ab-initio calculations of one-dimensional band structures of mixed-stack molecular crystals. Solid State Communications, 1997, 102, 589-594.	0.9	19

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73	Ab initio molecular dynamics calculations to study catalysis. International Journal of Quantum Chemistry, 1997, 61, 369-380.	1.0	33
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75	A Dynamical Density Functional Study on the Reaction of Ethylene with Cp2Zr(C2H5)+. Journal of the American Chemical Society, 1996, 118, 4434-4441.	6.6	125
76	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.	6.6	49
77	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.	6.6	149
78	First-Principles Investigation of Enantioselective Catalysis:Â Asymmetric Allylic Amination with Pd Complexes Bearing P,N-Ligands. Organometallics, 1996, 15, 4125-4132.	1.1	133
79	Struktur und Dynamik von Methanol in einem Zeolithen. Angewandte Chemie, 1996, 108, 187-189.	1.6	18
80	Interaction of water and methanol with a zeolite at high coverages. Chemical Physics Letters, 1996, 253, 448-455.	1.2	91
81	Structure and Dynamics of Methanol in a Zeolite. Angewandte Chemie International Edition in English, 1996, 35, 175-177.	4.4	88
82	Ab initiomolecular-dynamics study of diffusion and defects in solidLi3N. Physical Review B, 1996, 53, 9084-9091.	1.1	54
83	First-principles molecular-dynamics simulations for neutralp-chloranil and its radical anion. Physical Review B, 1996, 53, 12112-12120.	1.1	33
84	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.	2.9	63
85	Dynamics of beryllocene. Journal of Chemical Physics, 1995, 103, 683-690.	1.2	41
86	Reaction of Methane with Rh(PH3)2Cl: A Dynamical Density Functional Study. Journal of the American Chemical Society, 1995, 117, 12625-12634.	6.6	63
87	Electrostatic decoupling of periodic images of planeâ€waveâ€expanded densities and derived atomic point charges. Journal of Chemical Physics, 1995, 103, 7422-7428.	1.2	214
88	Finiteâ€temperature characterization of ferrocene from firstâ€principles molecular dynamics simulations. Journal of Chemical Physics, 1994, 100, 8194-8203.	1.2	49
89	Projector augmented-wave method. Physical Review B, 1994, 50, 17953-17979.	1.1	66,022
90	Improved tetrahedron method for Brillouin-zone integrations. Physical Review B, 1994, 49, 16223-16233.	1.1	5,977

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91	Fluxional Dynamics of Beryllocene. Journal of the American Chemical Society, 1994, 116, 11177-11178.	6.6	39
92	Hypothetical Carbon Modifications Derived from Zeolite Frameworks. Angewandte Chemie International Edition in English, 1993, 32, 701-703.	4.4	70
93	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.	2.9	2,932
94	First-principles calculations of self-diffusion constants in silicon. Physical Review Letters, 1993, 70, 2435-2438.	2.9	266
95	Adsorption and scanning-tunneling-microscope imaging of benzene on graphite andMoS2. Physical Review Letters, 1993, 70, 3263-3266.	2.9	136
96	First-principles calculations of hyperfine parameters. Physical Review B, 1993, 47, 4244-4255.	1.1	231
97	Native defects and self-compensation in ZnSe. Physical Review B, 1992, 45, 10965-10978.	1.1	273
98	Interacting loop-current model of superconducting networks. Journal of Low Temperature Physics, 1992, 88, 163-195.	0.6	18
99	Adiabaticity in first-principles molecular dynamics. Physical Review B, 1992, 45, 9413-9416.	1.1	296
100	Electronic structure of ordered and disordered Pd3Fe. Journal of Magnetism and Magnetic Materials, 1990, 87, 97-105.	1.0	15
101	First-principles calculations of diffusion coefficients: Hydrogen in silicon. Physical Review Letters, 1990, 64, 1401-1404.	2.9	84
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103	Daset al. reply. Physical Review Letters, 1990, 65, 2084-2084.	2.9	3
104	Generalized separable potentials for electronic-structure calculations. Physical Review B, 1990, 41, 5414-5416.	1.1	276
105	Electronic structure and Schottky-barrier heights of (111)NiSi2/Si A- and B-type interfaces. Physical Review Letters, 1989, 63, 1168-1171.	2.9	136
106	Electronic structure and properties ofNiSi2andCoSi2in the fluorite and adamantane structures. Physical Review B, 1987, 36, 2493-2503.	1.1	105