Peter Blchl

List of Publications by Citations

Source: https://exaly.com/author-pdf/3073530/peter-blochl-publications-by-citations.pdf
Version: 2024-04-10

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.
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	Projector augmented-wave method. *Physical Review B*, **1994**, 50, 17953-17979	3.3	50591
102	Improved tetrahedron method for Brillouin-zone integrations. *Physical Review B*, **1994**, 49, 16223-16233	3.3	5100
101	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
100	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
99	First-principles calculations of defects in oxygen-deficient silica exposed to hydrogen. *Physical Review B*, **2000**, 62, 6158-6179	3.3	299
98	Adiabaticity in first-principles molecular dynamics. *Physical Review B*, **1992**, 45, 9413-9416	3.3	279
97	Projector augmented wave method:ab initio molecular dynamics with full wave functions. *Bulletin of Materials Science*, **2003**, 26, 33-41	1.7	274
96	The interface between silicon and a high-k oxide. *Nature*, **2004**, 427, 53-6	50.4	266
95	Hydrogen Electrochemistry and Stress-Induced Leakage Current in Silica. *Physical Review Letters*, **1999**, 83, 372-375	7.4	265
94	Native defects and self-compensation in ZnSe. *Physical Review B*, **1992**, 45, 10965-10978	3.3	253
93	First-principles calculations of self-diffusion constants in silicon. *Physical Review Letters*, **1993**, 70, 2435-2438	7.4	240
92	Generalized separable potentials for electronic-structure calculations. *Physical Review B*, **1990**, 41, 5414-5416	3.3	236
91	First-principles calculations of hyperfine parameters. *Physical Review B*, **1993**, 47, 4244-4255	3.3	208
90	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
89	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
88	Electric-field-gradient calculations using the projector augmented wave method. *Physical Review B*, **1998**, 57, 14690-14697	3.3	167
87	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

86	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
85	Adsorption and scanning-tunneling-microscope imaging of benzene on graphite and MoS2. *Physical Review Letters*, **1993**, 70, 3263-3266	7.4	126
84	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
83	First-Principles Investigation of Enantioselective Catalysis: Asymmetric Allylic Amination with Pd Complexes Bearing P,N-Ligands. *Organometallics*, **1996**, 15, 4125-4132	3.8	118
82	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
81	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
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	Electronic structure and properties of NiSi2 and CoSi2 in the fluorite and adamantane structures. *Physical Review B*, **1987**, 36, 2493-2503	3.3	103
78	Nitrogen binding to the FeMo-cofactor of nitrogenase. *Journal of the American Chemical Society*, **2003**, 125, 15772-8	16.4	102
77	Hydrocarbon adsorption on Si(001): when does the Si dimer bond break?. *Surface Science*, **1997**, 374, 298-305	1.8	94
76	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
75	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
74	Solvation Effects on the SN2 Reaction between CH3Cl and Cl- in Water. *Journal of Physical Chemistry A*, **2001**, 105, 3300-3310	2.8	79
73	First-principles calculations of diffusion coefficients: Hydrogen in silicon. *Physical Review Letters*, **1990**, 64, 1401-1404	7.4	78
72	Interaction of water and methanol with a zeolite at high coverages. *Chemical Physics Letters*, **1996**, 253, 448-455	2.5	77
71	Structure and Dynamics of Methanol in a Zeolite. *Angewandte Chemie International Edition in English*, **1996**, 35, 175-177		75
70	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
69	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

68	In Situ Electrochemical Electron Microscopy Study of Oxygen Evolution Activity of Doped Manganite Perovskites. *Advanced Functional Materials*, **2012**, 22, 3378-3388	15.6	63
67	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
66	First-principles calculations of strontium on Si(001). *Physical Review B*, **2004**, 69,	3.3	58
65	Hypothetical Carbon Modifications Derived from Zeolite Frameworks. *Angewandte Chemie International Edition in English*, **1993**, 32, 701-703		58
64	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
63	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
62	Ab initio molecular-dynamics study of diffusion and defects in solid Li3N. *Physical Review B*, **1996**, 53, 9084-9091	3.3	48
61	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
60	Finite-temperature characterization of ferrocene from first-principles molecular dynamics simulations. *Journal of Chemical Physics*, **1994**, 100, 8194-8203	3.9	44
59	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
58	Activation and protonation of dinitrogen at the FeMo cofactor of nitrogenase. *Journal of Chemical Physics*, **2005**, 123, 074306	3.9	39
57	Towards an understanding of the workings of nitrogenase from DFT calculations. *ChemPhysChem*, **2005**, 6, 1724-6	3.2	36
56	Fluxional Dynamics of Beryllocene. *Journal of the American Chemical Society*, **1994**, 116, 11177-11178	16.4	35
55	Ab initio calculation of binding and diffusion of a Ga adatom on the GaAs (001)□(4□) surface. *Physical Review B*, **1998**, 58, 1499-1505	3.3	33
54	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
53	Dynamics of beryllocene. *Journal of Chemical Physics*, **1995**, 103, 683-690	3.9	33
52	First-principles molecular-dynamics simulations for neutral p-chloranil and its radical anion. *Physical Review B*, **1996**, 53, 12112-12120	3.3	33
51	Ab initio molecular dynamics with a continuum solvation model. *Journal of Chemical Physics*, **2003**, 118, 1089-1100	3.9	31

50	Ab initio molecular dynamics calculations to study catalysis. *International Journal of Quantum Chemistry*, **1997**, 61, 369-380	2.1	29
49	Model for acetylene reduction by nitrogenase derived from density functional theory. *Inorganic Chemistry*, **2005**, 44, 4568-75	5.1	29
48	Band alignment at the La2Hf2O7(001)Si interface. *Applied Physics Letters*, **2006**, 88, 202903	3.4	28
47	Density-matrix functionals from Green's functions. *Physical Review B*, **2013**, 88,	3.3	27
46	LDA+U calculated electronic and structural properties of NiO(001) and NiO(111) p(2×2) surfaces. *Computational Materials Science*, **2002**, 24, 192-198	3.2	27
45	First-principles molecular dynamics study of small molecules in zeolites. *Catalysis Today*, **1999**, 50, 501-509	3.3	27
44	Electronic structure of Pr1−xCaxMnO3. *Physical Review B*, **2017**, 95,	3.3	23
43	Temperature- and doping-dependent optical absorption in the small-polaron system Pr1−xCaxMnO3. *Physical Review B*, **2015**, 92,	3.3	23
42	Towards solvation simulations with a combined ab initio molecular dynamics and molecular mechanics approach. *Computational and Theoretical Chemistry*, **2000**, 506, 313-334		20
41	Ab-initio calculations of one-dimensional band structures of mixed-stack molecular crystals. *Solid State Communications*, **1997**, 102, 589-594	1.6	19
40	Interaction of NaCl with solid water. *Journal of Chemical Physics*, **2004**, 121, 9671-8	3.9	19
39	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
38	Struktur und Dynamik von Methanol in einem Zeolithen. *Angewandte Chemie*, **1996**, 108, 187-189	3.6	17
37	Evolution of Hot Polaron States with a Nanosecond Lifetime in a Manganite Perovskite. *Advanced Energy Materials*, **2017**, 7, 1602174	21.8	16
36	Reduced density-matrix functionals applied to the Hubbard dimer. *Physical Review B*, **2016**, 93,	3.3	16
35	Reduced density-matrix functionals from many-particle theory. *European Physical Journal: Special Topics*, **2017**, 226, 2677-2692	2.3	16
34	Chemistry of La on the Si(001) surface from first principles. *Physical Review B*, **2004**, 70,	3.3	16
33	Second-generation wave-function thermostat for ab initio molecular dynamics. *Physical Review B*, **2002**, 65,	3.3	16

32	Interacting loop-current model of superconducting networks. *Journal of Low Temperature Physics*, **1992**, 88, 163-195	1.3	16
31	Method to include explicit correlations into density-functional calculations based on density-matrix functional theory. *Physical Review B*, **2011**, 84,	3.3	15
30	Electronic structure of ordered and disordered Pd3Fe. *Journal of Magnetism and Magnetic Materials* , **1990**, 87, 97-105	2.8	15
29	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
28	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
27	Electronic Structure Methods: Augmented Waves, Pseudopotentials and The Projector Augmented Wave Method **2005**, 93-119		11
26	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
25	Hybrid density functional theory benchmark study on lithium manganese oxides. *Physical Review B*, **2020**, 101,	3.3	10
24	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
23	Ab Initio Molecular Dynamics with the Projector Augmented Wave Method. *ACS Symposium Series*, **1996**, 54-69	0.4	9
22	Dynamic observation of manganese adatom mobility at perovskite oxide catalyst interfaces with water. *Communications Materials*, **2020**, 1,	6	9
21	Dynamical dimer method for the determination of transition states with ab initio molecular dynamics. *Journal of Chemical Physics*, **2008**, 128, 044107	3.9	8
20	Chemical Involvement of Solvent Water Molecules in Elementary Steps of the Fenton Oxidation Reaction. *Angewandte Chemie*, **2001**, 113, 2977-2979	3.6	7
19	Phase boundary of superconducting networks: A new approximation scheme. *Physical Review B*, **1990**, 42, 76-79	3.3	7
18	A Review of Density Functional Models for the Description of Fe(II) Spin-Crossover Complexes. *Molecules*, **2020**, 25,	4.8	6
17	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
16	Ab-initio simulations on growth and interface properties of epitaxial oxides on silicon. *Microelectronic Engineering*, **2005**, 80, 402-407	2.5	5
15	Molecular Reaction Modeling from Ab-Initio Molecular Dynamics. *ACS Symposium Series*, **1999**, 88-99	0.4	5

List of Publications

14	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
13	Evolution of the magnetic and polaronic order of Pr1/2Ca1/2MnO3 following an ultrashort light pulse. *Physical Review B*, **2020**, 102,	3.3	3
12	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
11	Relaxation of photoexcitations in polaron-induced magnetic microstructures. *Physical Review B*, **2018**, 97,	3.3	3
10	Surface resonance of the (2□1) reconstructed lanthanum hexaboride (001)-cleavage plane: A combined STM and DFT study. *Physical Review B*, **2019**, 100,	3.3	3
9	Das et al. reply. *Physical Review Letters*, **1990**, 65, 2084	7.4	3
8	Taming the ground-state and optical properties of transition metal oxides. *Computational Materials Science*, **2000**, 17, 146-150	3.2	2
7	Orbital-order phase transition in Pr1□CaxMnO3 probed by photovoltaics. *Physical Review B*, **2021**, 103,	3.3	2
6	Ultrafast spin-nematic and ferroelectric phase transitions induced by femtosecond light pulses. *Physical Review B*, **2020**, 102,	3.3	1
5	Adaptive cluster approximation for reduced density-matrix functional theory. *Physical Review B*, **2018**, 97,	3.3	1
4	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
3	Theoretical study of interaction of laser with diatomic molecules using the Basis Generator Method. *Journal of Physics: Conference Series*, **2009**, 194, 032052	0.3	
2	Molecular design of interfaces based on density-functional simulations. *Zeitschrift Fur Anorganische Und Allgemeine Chemie*, **2006**, 632, 2075-2075	1.3	
1	Modeling of Growth of High-□Oxides on Semiconductors **2007**, 165-179		