Juerg Hutter

List of Publications by Year in Descending Order

168 papers	21,341 citations	60 h-index	145 g-index
174 ext. papers	23,950 ext. citations	5.4 avg, IF	7.07 L-index

#	Paper	IF	Citations
168	Double-hybrid density functionals for the condensed phase: Gradients, stress tensor, and auxiliary-density matrix method acceleration.. *Journal of Chemical Physics*, **2022**, 156, 074107	3.9	1
167	Towards electronic structure-based ab-initio molecular dynamics simulations with hundreds of millions of atoms. *Parallel Computing*, **2022**, 111, 102920	1	3
166	Efficient and low-scaling linear-response time-dependent density functional theory implementation for core-level spectroscopy of large and periodic systems. *Physical Chemistry Chemical Physics*, **2021**, 23, 4736-4746	3.6	6
165	First-principles correction scheme for linear-response time-dependent density functional theory calculations of core electronic states. *Journal of Chemical Physics*, **2021**, 155, 034108	3.9	3
164	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. *Journal of Chemical Physics*, **2020**, 152, 194103	3.9	421
163	MP2- and RPA-Based Ab Initio Molecular Dynamics and Monte Carlo Sampling **2020**, 523-543		
162	Modelling electrochemical systems with finite field molecular dynamics. *JPhys Energy*, **2020**, 2, 032005	4.9	32
161	Quantifying the hydration structure of sodium and potassium ions: taking additional steps on Jacob☺ Ladder. *Physical Chemistry Chemical Physics*, **2020**, 22, 10641-10652	3.6	24
160	Double-Hybrid DFT Functionals for the Condensed Phase: Gaussian and Plane Waves Implementation and Evaluation. *Molecules*, **2020**, 25,	4.8	6
159	Coupling of Surface Chemistry and Electric Double Layer at TiO Electrochemical Interfaces. *Journal of Physical Chemistry Letters*, **2019**, 10, 3871-3876	6.4	36
158	Stable and tunable phosphonic acid dipole layer for band edge engineering of photoelectrochemical and photovoltaic heterojunction devices. *Energy and Environmental Science*, **2019**, 12, 1901-1909	35.4	32
157	DBCSR: A Library for Dense Matrix Multiplications on Distributed GPU-Accelerated Systems **2019**,		1
156	Toward GW Calculations on Thousands of Atoms. *Journal of Physical Chemistry Letters*, **2018**, 9, 306-312	6.4	65
155	Second generation Car-Parrinello MD: application to the h-BN/Rh(111) nanomesh. *European Physical Journal B*, **2018**, 91, 1	1.2	5
154	MP2- and RPA-Based Ab Initio Molecular Dynamics and Monte Carlo Sampling **2018**, 1-21		1
153	Large-Scale Computation of Nuclear Magnetic Resonance Shifts for Paramagnetic Solids Using CP2K. *Journal of Chemical Theory and Computation*, **2018**, 14, 377-394	6.4	25
152	First-Principles Simulations of an Aqueous CO/Pt(111) Interface. *Journal of Physical Chemistry C*, **2018**, 122, 24068-24076	3.8	23

151	Exploring the Limitation of Molecular Water Oxidation Catalysts. *Journal of Physical Chemistry C*, **2018**, 122, 12404-12412	3.8	27
150	Local Fitting of the Kohn-Sham Density in a Gaussian and Plane Waves Scheme for Large-Scale Density Functional Theory Simulations. *Journal of Chemical Theory and Computation*, **2017**, 13, 2202-2214	6.4	5
149	Insight into (Co)Pyrphyrin Adsorption on Au(111): Effects of Herringbone Reconstruction and Dynamics of Metalation. *Journal of Physical Chemistry C*, **2017**, 121, 11416-11427	3.8	13
148	Post-Synthesis Amine Borane Functionalization of a Metal-Organic Framework and Its Unusual Chemical Hydrogen Release Phenomenon. *Chemistry - A European Journal*, **2017**, 23, 8823-8828	4.8	5
147	Fast evaluation of solid harmonic Gaussian integrals for local resolution-of-the-identity methods and range-separated hybrid functionals. *Journal of Chemical Physics*, **2017**, 146, 034105	3.9	8
146	The impact of metalation on adsorption geometry, electronic level alignment and UV-stability of organic macrocycles on TiO(110). *Nanoscale*, **2017**, 9, 8756-8763	7.7	5
145	Mapping the Free Energy of Lithium Solvation in the Protic Ionic Liquid Ethylammonuim Nitrate: A Metadynamics Study. *ChemSusChem*, **2017**, 10, 3083-3090	8.3	7
144	Increasing the Efficiency of Sparse Matrix-Matrix Multiplication with a 2.5D Algorithm and One-Sided MPI **2017**,		5
143	Periodic GW calculations in the Gaussian and plane-waves scheme. *Physical Review B*, **2017**, 95,	3.3	23
142	Mass density fluctuations in quantum and classical descriptions of liquid water. *Journal of Chemical Physics*, **2017**, 146, 244501	3.9	37
141	GW in the Gaussian and Plane Waves Scheme with Application to Linear Acenes. *Journal of Chemical Theory and Computation*, **2016**, 12, 3623-35	6.4	71
140	GPU-Accelerated Sparse Matrix□Matrix Multiplication for Linear Scaling Density Functional Theory **2016**, 173-190		18
139	Large-Scale Cubic-Scaling Random Phase Approximation Correlation Energy Calculations Using a Gaussian Basis. *Journal of Chemical Theory and Computation*, **2016**, 12, 5851-5859	6.4	47
138	From porphyrins to pyrphyrins: adsorption study and metalation of a molecular catalyst on Au(111). *Nanoscale*, **2016**, 8, 7958-68	7.7	25
137	Computing the Kirkwood g-Factor by Combining Constant Maxwell Electric Field and Electric Displacement Simulations: Application to the Dielectric Constant of Liquid Water. *Journal of Physical Chemistry Letters*, **2016**, 7, 2696-701	6.4	50
136	Formation and properties of a terpyridine-based 2D MOF on the surface of water. *2D Materials*, **2016**, 3, 025026	5.9	4
135	Computational Investigation and Design of Cobalt Aqua Complexes for Homogeneous Water Oxidation. *Journal of Physical Chemistry C*, **2016**, 120, 7966-7975	3.8	31
134	Liquid Water through Density-Functional Molecular Dynamics: Plane-Wave vs Atomic-Orbital Basis Sets. *Journal of Chemical Theory and Computation*, **2016**, 12, 3456-62	6.4	19

133	Thermal Effects on CH3NH3PbI3 Perovskite from Ab Initio Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2015**, 119, 8991-8997	3.8	101
132	Wetting of water on hexagonal boron nitride@Rh(111): a QM/MM model based on atomic charges derived for nano-structured substrates. *Physical Chemistry Chemical Physics*, **2015**, 17, 14307-16	3.6	29
131	Dividing a complex reaction involving a hypervalent iodine reagent into three limiting mechanisms by ab initio molecular dynamics. *Journal of Computational Chemistry*, **2015**, 36, 785-94	3.5	29
130	Non-innocent adsorption of Co-pyrphyrin on rutile(110). *Physical Chemistry Chemical Physics*, **2015**, 17, 22846-54	3.6	18
129	Enabling simulation at the fifth rung of DFT: Large scale RPA calculations with excellent time to solution. *Computer Physics Communications*, **2015**, 187, 120-129	4.2	35
128	Forces and stress in second order Møller-Plesset perturbation theory for condensed phase systems within the resolution-of-identity Gaussian and plane waves approach. *Journal of Chemical Physics*, **2015**, 143, 102803	3.9	50
127	Probing the structural and dynamical properties of liquid water with models including non-local electron correlation. *Journal of Chemical Physics*, **2015**, 143, 054506	3.9	78
126	Building Blocks for Two-Dimensional Metal–Organic Frameworks Confined at the Air–Water Interface: An Ab Initio Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2015**, 119, 4023-4030	3.8	12
125	Functionalization of CeO2(1 1 1) by Deposition of Small Ni Clusters: Effects on CO2 Adsorption and O Vacancy Formation. *ChemCatChem*, **2015**, 7, 625-634	5.2	27
124	Site-selective adsorption of phthalocyanine on h-BN/Rh(111) nanomesh. *Physical Chemistry Chemical Physics*, **2014**, 16, 12374-84	3.6	39
123	Dielectric properties of water ice, the ice Ih/XI phase transition, and an assessment of density functional theory. *Journal of Physical Chemistry B*, **2014**, 118, 590-6	3.4	29
122	Control of molecular organization and energy level alignment by an electronically nanopatterned boron nitride template. *ACS Nano*, **2014**, 8, 430-42	16.7	68
121	Synthesis and hydrogen adsorption properties of internally polarized 2,6-azulenedicarboxylate based metal–organic frameworks. *Journal of Materials Chemistry A*, **2014**, 2, 18823-18830	13	22
120	Describing the chemical bonding in C70 and C70O3 – A quantum chemical topology study. *Chemical Physics*, **2014**, 433, 22-30	2.3	8
119	Correction to "Bulk Liquid Water at Ambient Temperature and Pressure from MP2 Theory". *Journal of Physical Chemistry Letters*, **2014**, 5, 3066-7	6.4	16
118	Sparse matrix multiplication: The distributed block-compressed sparse row library. *Parallel Computing*, **2014**, 40, 47-58	1	94
117	Dehalogenation and coupling of a polycyclic hydrocarbon on an atomically thin insulator. *ACS Nano*, **2014**, 8, 6571-9	16.7	42
116	Electron transfer modifies chemical properties of C70 fullerene surface: An ab initio molecular dynamics study of C70O3 molozonides doped with light atoms. *Chemical Physics Letters*, **2014**, 605-606, 93-97	2.5	2

115	cp2k: atomistic simulations of condensed matter systems. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 15-25	7.9	1578
114	Chemical Reactions on Metal-supported Hexagonal Boron Nitride Investigated with Density Functional Theory. *Chimia*, **2014**, 68, 596-601	1.3	9
113	Significant substituent effect on the anomerization of pyranosides: mechanism of anomerization and synthesis of a 1,2-cis glucosamine oligomer from the 1,2-trans anomer. *Chemistry - A European Journal*, **2014**, 20, 124-32	4.8	20
112	Raman spectra from ab initio molecular dynamics and its application to liquid S-methyloxirane. *Journal of Chemical Physics*, **2014**, 141, 094503	3.9	43
111	Hexagonal boron nitride on transition metal surfaces. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	85
110	Bulk Liquid Water at Ambient Temperature and Pressure from MP2 Theory. *Journal of Physical Chemistry Letters*, **2013**, 4, 3753-3759	6.4	117
109	Impact of donor-acceptor functionalization on the properties of linearly π-conjugated oligomers: establishing quantitative relationships for the substituent and substituent cooperative effect based on quantum chemical calculations. *Journal of Organic Chemistry*, **2013**, 78, 12681-9	4.2	7
108	Efficient Linear-Scaling Density Functional Theory for Molecular Systems. *Journal of Chemical Theory and Computation*, **2013**, 9, 4421-7	6.4	23
107	Moiré beatings in graphene on Ru(0001). *Physical Review B*, **2013**, 88,	3.3	35
106	Coverage Effect of the CO2 Adsorption Mechanisms on CeO2(111) by First Principles Analysis. *Journal of Physical Chemistry C*, **2013**, 117, 1701-1711	3.8	79
105	Structural and electronic properties of a large-scale Moiré pattern of hexagonal boron nitride on Cu(111) studied with density functional theory. *Nanoscale*, **2013**, 5, 5589-95	7.7	30
104	Nonlocal van der Waals functionals: the case of rare-gas dimers and solids. *Journal of Chemical Physics*, **2013**, 138, 204103	3.9	37
103	Electron Correlation in the Condensed Phase from a Resolution of Identity Approach Based on the Gaussian and Plane Waves Scheme. *Journal of Chemical Theory and Computation*, **2013**, 9, 2654-71	6.4	99
102	Simulation of Adsorption Processes at Metallic Interfaces: An Image Charge Augmented QM/MM Approach. *Journal of Chemical Theory and Computation*, **2013**, 9, 5086-97	6.4	56
101	Second-Order Møller-Plesset Perturbation Theory in the Condensed Phase: An Efficient and Massively Parallel Gaussian and Plane Waves Approach. *Journal of Chemical Theory and Computation*, **2012**, 8, 4177-88	6.4	106
100	Chiral distortion of confined ice oligomers (N = 5,6). *Langmuir*, **2012**, 28, 15246-50	4	10
99	Local Disorder in Lithium Imide from Density Functional Simulation and NMR Spectroscopy. *Journal of Physical Chemistry C*, **2012**, 116, 18577-18583	3.8	5
98	Linear Scaling Self-Consistent Field Calculations with Millions of Atoms in the Condensed Phase. *Journal of Chemical Theory and Computation*, **2012**, 8, 3565-73	6.4	111

97	Boron nitride on Cu(111): an electronically corrugated monolayer. *Nano Letters*, **2012**, 12, 5821-8	11.5	168
96	CarParrinello molecular dynamics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 604-612	7.9	94
95	Real-world predictions from ab initio molecular dynamics simulations. *Topics in Current Chemistry*, **2012**, 307, 109-53		74
94	Nano-ice models for the water aggregates observed on the h-BN/Rh(111) nanomesh. *Journal of Physics Condensed Matter*, **2012**, 24, 445002	1.8	3
93	Endocyclic cleavage in glycosides with 2,3-trans cyclic protecting groups. *Journal of the American Chemical Society*, **2011**, 133, 5610-9	16.4	61
92	Investigation of -BN/Rh(111) Nanomesh Interacting with Water and Atomic Hydrogen. *Chimia*, **2011** , 65, 256-259	1.3	7
91	Semiempirical self-consistent polarization description of bulk water, the liquid-vapor interface, and cubic ice. *Journal of Physical Chemistry A*, **2011**, 115, 6046-53	2.8	21
90	Investigation of Boron Nitride Nanomesh Interacting with Water. *Journal of Physical Chemistry C*, **2011**, 115, 13685-13692	3.8	39
89	Comparative study of the nature of chemical bonding of corrugated graphene on Ru(0001) and Rh(111) by electronic structure calculations. *Surface Science*, **2011**, 605, 1360-1368	1.8	56
88	On the emergence of molecular structure. *Physical Review A*, **2011**, 83,	2.6	44
87	Extracting elements of molecular structure from the all-particle wave function. *Journal of Chemical Physics*, **2011**, 135, 204302	3.9	36
86	An atomistic picture of the regeneration process in dye sensitized solar cells. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 4830-3	11.5	82
85	Protonation-Dependent Binding of Ruthenium Bipyridyl Complexes to the Anatase(101) Surface. *Journal of Physical Chemistry C*, **2010**, 114, 8398-8404	3.8	96
84	Auxiliary Density Matrix Methods for Hartree-Fock Exchange Calculations. *Journal of Chemical Theory and Computation*, **2010**, 6, 2348-64	6.4	321
83	Nano-ice on boron nitride nanomesh: accessing proton disorder. *ChemPhysChem*, **2010**, 11, 399-403	3.2	31
82	Nanotexture Switching of Single-Layer Hexagonal Boron Nitride on Rhodium by Intercalation of Hydrogen Atoms. *Angewandte Chemie*, **2010**, 122, 6256-6260	3.6	2
81	Nanotexture switching of single-layer hexagonal boron nitride on rhodium by intercalation of hydrogen atoms. *Angewandte Chemie - International Edition*, **2010**, 49, 6120-4	16.4	62
80	A QM/MM investigation of thymine dimer radical anion splitting catalyzed by DNA photolyase. *ChemPhysChem*, **2009**, 10, 400-10	3.2	67

79	Low-Barrier Pathway for endo-Cleavage Induced Anomerization of Pyranosides with N-Benzyl-2,3-trans-oxazolidinone Groups. *European Journal of Organic Chemistry*, **2009**, 2009, 1127-1131	3.2	21
78	Isobaric-isothermal molecular dynamics simulations utilizing density functional theory: an assessment of the structure and density of water at near-ambient conditions. *Journal of Physical Chemistry B*, **2009**, 113, 11959-64	3.4	302
77	Magnetic linear response properties calculations with the Gaussian and augmented-plane-wave method. *Journal of Chemical Physics*, **2009**, 131, 014106	3.9	45
76	Accurate Hartree-Fock energy of extended systems using large Gaussian basis sets. *Physical Review B*, **2009**, 80,	3.3	42
75	Robust Periodic Hartree-Fock Exchange for Large-Scale Simulations Using Gaussian Basis Sets. *Journal of Chemical Theory and Computation*, **2009**, 5, 3010-21	6.4	189
74	A Scheme for the Evaluation of Electron Delocalization and Conjugation Efficiency in Linearly Conjugated Systems. *Journal of Chemical Theory and Computation*, **2009**, 5, 506-14	6.4	25
73	Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods **2009**,		990
72	Ab initio molecular dynamics using hybrid density functionals. *Journal of Chemical Physics*, **2008**, 128, 214104	3.9	182
71	Computational study of thymine dimer radical anion splitting in the self-repair process of duplex DNA. *Journal of the American Chemical Society*, **2008**, 130, 3443-50	16.4	59
70	Beyond isotropic tumbling models: nuclear spin relaxation in liquids from first principles. *ChemPhysChem*, **2008**, 9, 2313-6	3.2	26
69	Car-Parrinello Molecular Dynamics Simulations of CaCl2 Aqueous Solutions. *Journal of Chemical Theory and Computation*, **2008**, 4, 779-89	6.4	63
68	Notes on "Ewald summation of electrostatic multipole interactions up to quadrupolar level" [J. Chem. Phys. 119, 7471 (2003)]. *Journal of Chemical Physics*, **2008**, 129, 074102	3.9	42
67	Direct energy functional minimization under orthogonality constraints. *Journal of Chemical Physics*, **2008**, 128, 084113	3.9	45
66	A smooth script-l1-norm sparseness function for orbital based linear scaling total energy minimization. *Journal of Chemical Physics*, **2008**, 128, 064107	3.9	13
65	Atomistic simulations of a solid/liquid interface: a combined force field and first principles approach to the structure and dynamics of acetonitrile near an anatase surface. *Journal of Physics Condensed Matter*, **2008**, 20, 064206	1.8	17
64	Inner-shell spectroscopy by the Gaussian and augmented plane wave method. *Physical Chemistry Chemical Physics*, **2007**, 9, 1599-610	3.6	69
63	Gaussian basis sets for accurate calculations on molecular systems in gas and condensed phases. *Journal of Chemical Physics*, **2007**, 127, 114105	3.9	2003
62	Towards a rational design of ruthenium CO2 hydrogenation catalysts by Ab initio metadynamics. *Chemistry - A European Journal*, **2007**, 13, 6828-40	4.8	60

61	Molecular dynamics simulation of liquid water: hybrid density functionals. *Journal of Physical Chemistry B*, **2006**, 110, 3685-91	3.4	222
60	Simulating fluid-phase equilibria of water from first principles. *Journal of Physical Chemistry A*, **2006**, 110, 640-6	2.8	125
59	Density functional embedding for molecular systems. *Chemical Physics Letters*, **2006**, 421, 16-20	2.5	71
58	Ionic liquids from Car-Parrinello simulations, part I: liquid AlCl3. *Journal of Physical Chemistry B*, **2006**, 110, 11475-80	3.4	29
57	A density-functional approach to polarizable models: a Kim-Gordon response density interaction potential for molecular simulations. *Journal of Chemical Physics*, **2005**, 123, 074108	3.9	12
56	CPMD: Car-Parrinello molecular dynamics. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2005**, 220,	1	26
55	Dual-level parallelism for ab initio molecular dynamics: Reaching teraflop performance with the CPMD code. *Parallel Computing*, **2005**, 31, 1-17	1	51
54	Quickstep: Fast and accurate density functional calculations using a mixed Gaussian and plane waves approach. *Computer Physics Communications*, **2005**, 167, 103-128	4.2	3322
53	The influence of temperature and density functional models in ab initio molecular dynamics simulation of liquid water. *Journal of Chemical Physics*, **2005**, 122, 14515	3.9	417
52	Isobaric-isothermal monte carlo simulations from first principles: application to liquid water at ambient conditions. *ChemPhysChem*, **2005**, 6, 1894-901	3.2	93
51	Car-Parrinello molecular dynamics on massively parallel computers. *ChemPhysChem*, **2005**, 6, 1788-93	3.2	93
50	Car-Parrinello molecular dynamics study of the initial dinitrogen reduction step in Sellmann-type nitrogenase model complexes. *Chemistry - A European Journal*, **2005**, 11, 574-83	4.8	28
49	Toward a Monte Carlo program for simulating vapor□liquid phase equilibria from first principles. *Computer Physics Communications*, **2005**, 169, 289-294	4.2	25
48	Ground and Excited State Density Functional Calculations with the Gaussian and Augmented-Plane-Wave Method. *Chimia*, **2005**, 59, 499-503	1.3	38
47	Solvent effects on electronic properties from Wannier functions in a dimethyl sulfoxide/water mixture. *Journal of Chemical Physics*, **2004**, 121, 5133-42	3.9	79
46	HYDROPHOBIC HYDRATION FROM CAR□PARRINELLO SIMULATIONS. *International Journal of Modern Physics B*, **2004**, 18, 1951-1962	1.1	26
45	Computational approaches to activity in rhodium-catalysed hydroformylation. *Chemistry - A European Journal*, **2004**, 10, 2435-44	4.8	48
44	A photochemical activation scheme of inert dinitrogen by dinuclear Ru(II) and Fe(II) complexes. *Chemistry - A European Journal*, **2004**, 10, 4443-53	4.8	40

43	Hartree–Fock exchange in time dependent density functional theory: application to charge transfer excitations in solvated molecular systems. *Chemical Physics Letters*, **2004**, 394, 141-146	2.5	49
42	s-Tetrazine in Aqueous Solution: A Density Functional Study of Hydrogen Bonding and Electronic Excitations. *Journal of Physical Chemistry A*, **2004**, 108, 2044-2052	2.8	28
41	Liquid Water from First Principles:´ Investigation of Different Sampling Approaches. *Journal of Physical Chemistry B*, **2004**, 108, 12990-12998	3.4	309
40	Large Scale Density Functional Calculations. *Lecture Notes in Computational Science and Engineering* , **2004**, 195-204	0.3	1
39	Time dependent density functional theory study of charge-transfer and intramolecular electronic excitations in acetone–water systems. *Journal of Chemical Physics*, **2003**, 119, 12417-12431	3.9	128
38	QM/MM Car-Parrinello molecular dynamics study of the solvent effects on the ground state and on the first excited singlet state of acetone in water. *ChemPhysChem*, **2003**, 4, 1177-82	3.2	105
37	Excited state geometries within time-dependent and restricted open-shell density functional theories. *Computational and Theoretical Chemistry*, **2003**, 630, 163-175		21
36	Excited state nuclear forces from the Tamm–Dancoff approximation to time-dependent density functional theory within the plane wave basis set framework. *Journal of Chemical Physics*, **2003**, 118, 3928-3934	3.9	154
35	An efficient orbital transformation method for electronic structure calculations. *Journal of Chemical Physics*, **2003**, 118, 4365-4369	3.9	362
34	The structure of a DMSO–water mixture from Car–Parrinello simulations. *Chemical Physics Letters*, **2002**, 364, 497-502	2.5	54
33	Comment on "Dissociation of water under pressure". *Physical Review Letters*, **2002**, 89, 199601; author reply 199602	7.4	8
32	Classical polarizable force fields parametrized from ab initio calculations. *Journal of Chemical Physics*, **2002**, 117, 1416-1433	3.9	55
31	Polarized atomic orbitals for linear scaling methods. *Journal of Chemical Physics*, **2002**, 116, 1800-1810	3.9	18
30	Time and Length Scales in ab initio Molecular Dynamics. *Lecture Notes in Physics*, **2002**, 413-442	0.8	2
29	Structural and electronic properties of Co-corrole, Co-corrin, and Co-porphyrin. *Inorganic Chemistry*, **2001**, 40, 11-7	5.1	74
28	Ab initio analysis of proton transfer dynamics in (H2O)3H+. *Chemical Physics Letters*, **2000**, 321, 225-230	2.5	50
27	General and efficient algorithms for obtaining maximally localized Wannier functions. *Physical Review B*, **2000**, 61, 10040-10048	3.3	229
26	Microsolvation and Chemical Reactivity of Sodium and Water Clusters. *Journal of the American Chemical Society*, **2000**, 122, 4837-4838	16.4	58

25	The Gaussian and augmented-plane-wave density functional method for ab initio molecular dynamics simulations. *Theoretical Chemistry Accounts*, **1999**, 103, 124-140	1.9	435
24	The nature of the hydrated excess proton in water. *Nature*, **1999**, 397, 601-604	50.4	1399
23	A comparative study of O2, CO, and NO binding to iron porphyrin. *International Journal of Quantum Chemistry*, **1998**, 69, 31-35	2.1	66
22	CO Oxidation on Pt(111): An Ab Initio Density Functional Theory Study. *Physical Review Letters*, **1998**, 80, 3650-3653	7.4	588
21	Understanding the Nature of Water Bound to Solid Acid Surfaces. Ab Initio Simulation on HSAPO-34. *Journal of the American Chemical Society*, **1998**, 120, 8512-8516	16.4	75
20	Molecular dynamics in low-spin excited states. *Journal of Chemical Physics*, **1998**, 108, 4060-4069	3.9	219
19	Equilibrium Geometries and Electronic Structure of Iron Porphyrin Complexes: A Density Functional Study. *Journal of Physical Chemistry A*, **1997**, 101, 8914-8925	2.8	347
18	Density Functional Theory-Based Molecular Dynamics Simulation of Acid-Catalyzed Chemical Reactions in Liquid Trioxane. *Journal of the American Chemical Society*, **1997**, 119, 7218-7229	16.4	82
17	Ab initio molecular dynamics simulation of methanol adsorbed in chabazite. *Chemical Physics Letters*, **1997**, 266, 397-402	2.5	85
16	A hybrid Gaussian and plane wave density functional scheme. *Molecular Physics*, **1997**, 92, 477-487	1.7	633
15	Ab initio molecular dynamics simulation of liquid water: Comparison of three gradient-corrected density functionals. *Journal of Chemical Physics*, **1996**, 105, 1142-1152	3.9	562
14	Nonempirical Calculations of a Hydrated RNA Duplex. *Journal of the American Chemical Society*, **1996**, 118, 8710-8712	16.4	40
13	Response Function Basis Sets: Application to Density Functional Calculations. *The Journal of Physical Chemistry*, **1996**, 100, 6231-6235		27
12	A First Principles Investigation of the Structure of a Bacteriochlorophyll Crystal. *Journal of the American Chemical Society*, **1996**, 118, 7847-7848	16.4	20
11	Integrating the Car Parrinello equations. III. Techniques for ultrasoft pseudopotentials. *Journal of Chemical Physics*, **1995**, 102, 859-871	3.9	48
10	C61H2 in Molecular and Solid Phases: Density-Functional Approach to Structural and Electronic Properties. *The Journal of Physical Chemistry*, **1995**, 99, 4008-4014		17
9	The molecular and electronic structure of s-tetrazine in the ground and first excited state: A theoretical investigation. *Journal of Chemical Physics*, **1995**, 103, 7048-7057	3.9	31
8	Structure and bonding in cisplatin and other Pt(II) complexes. *Chemical Physics Letters*, **1995**, 234, 50-56	2.5	82

7	Carboplatin versus cisplatin: density functional approach to their molecular properties. *Chemical Physics Letters*, **1995**, 246, 469-474	2.5	25
6	Exponential transformation of molecular orbitals. *Journal of Chemical Physics*, **1994**, 101, 3862-3865	3.9	29
5	Density-Functional-Theory-Based Molecular Dynamics Study of 1,3,5-Trioxane and 1,3-Dioxolane Protolysis. *Journal of the American Chemical Society*, **1994**, 116, 11251-11255	16.4	17
4	Structures and vibrational frequencies of the carbon molecules C2-C18 calculated by density functional theory. *Journal of the American Chemical Society*, **1994**, 116, 750-756	16.4	184
3	Electronic structure optimization in plane-wave-based density functional calculations by direct inversion in the iterative subspace. *Computational Materials Science*, **1994**, 2, 244-248	3.2	134
2	The molecular structure of C6: A theoretical investigation. *Journal of Chemical Physics*, **1994**, 101, 2213-2216	3.9	37
1	The structure of n-fold negatively charged C60 (n = 1, 2, 6). *International Journal of Quantum Chemistry*, **1993**, 46, 81-86	2.1	10