Juerg Hutter

List of Publications by Year
in descending order

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166 papers	26,769 citations	19636 61 h-index	6294 158 g-index
174 all docs	174 docs citations	174 times ranked	17237 citing authors

#	Article	IF	Citations
1	Quickstep: Fast and accurate density functional calculations using a mixed Gaussian and plane waves approach. Computer Physics Communications, 2005, 167, 103-128.	3.0	4,200
2	Gaussian basis sets for accurate calculations on molecular systems in gas and condensed phases. Journal of Chemical Physics, 2007, 127, 114105.	1.2	2,793
3	<scp>cp2k:</scp> atomistic simulations of condensed matter systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 15-25.	6.2	2,049
4	The nature of the hydrated excess proton in water. Nature, 1999, 397, 601-604.	13.7	1,587
5	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194103.	1.2	1,371
6	A hybrid Gaussian and plane wave density functional scheme. Molecular Physics, 1997, 92, 477-487.	0.8	881
7	CO Oxidation on Pt(111): AnAb InitioDensity Functional Theory Study. Physical Review Letters, 1998, 80, 3650-3653.	2.9	675
8	Ab initio molecular dynamics simulation of liquid water: Comparison of three gradientâ€corrected density functionals. Journal of Chemical Physics, 1996, 105, 1142-1152.	1.2	597
9	The Gaussian and augmented-plane-wave density functional method for ab initio molecular dynamics simulations. Theoretical Chemistry Accounts, 1999, 103, 124-140.	0.5	513
10	An efficient orbital transformation method for electronic structure calculations. Journal of Chemical Physics, 2003, 118, 4365-4369.	1.2	460
11	The influence of temperature and density functional models in ab initio molecular dynamics simulation of liquid water. Journal of Chemical Physics, 2005, 122, 014515.	1.2	444
12	Auxiliary Density Matrix Methods for Hartreeâ^'Fock Exchange Calculations. Journal of Chemical Theory and Computation, 2010, 6, 2348-2364.	2.3	438
13	Equilibrium Geometries and Electronic Structure of Ironâ^'Porphyrin Complexes:â€‰ A Density Functional Study. Journal of Physical Chemistry A, 1997, 101, 8914-8925.	1.1	362
14	Liquid Water from First Principles:Â Investigation of Different Sampling Approaches. Journal of Physical Chemistry B, 2004, 108, 12990-12998.	1.2	327
15	Isobaricâ^'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, 11959-11964.	1.2	327
16	General and efficient algorithms for obtaining maximally localized Wannier functions. Physical Review B, 2000, 61, 10040-10048.	1.1	272
17	Robust Periodic Hartreeâ^'Fock Exchange for Large-Scale Simulations Using Gaussian Basis Sets. Journal of Chemical Theory and Computation, 2009, 5, 3010-3021.	2.3	254
18	Molecular dynamics in low-spin excited states. Journal of Chemical Physics, 1998, 108, 4060-4069.	1.2	249

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19	Molecular Dynamics Simulation of Liquid Water:Â Hybrid Density Functionalsâ€. Journal of Physical Chemistry B, 2006, 110, 3685-3691.	1.2	242
20	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.	6.6	213
21	Ab initio molecular dynamics using hybrid density functionals. Journal of Chemical Physics, 2008, 128, 214104.	1.2	207
22	Boron Nitride on Cu(111): An Electronically Corrugated Monolayer. Nano Letters, 2012, 12, 5821-5828.	4.5	187
23	Excited state nuclear forces from the Tammâ€“Dancoff approximation to time-dependent density functional theory within the plane wave basis set framework. Journal of Chemical Physics, 2003, 118, 3928-3934.	1.2	173
24	Electronic structure optimization in plane-wave-based density functional calculations by direct inversion in the iterative subspace. Computational Materials Science, 1994, 2, 244-248.	1.4	147
25	Sparse matrix multiplication: The distributed block-compressed sparse row library. Parallel Computing, 2014, 40, 47-58.	1.3	143
26	Linear Scaling Self-Consistent Field Calculations with Millions of Atoms in the Condensed Phase. Journal of Chemical Theory and Computation, 2012, 8, 3565-3573.	2.3	138
27	Time dependent density functional theory study of charge-transfer and intramolecular electronic excitations in acetoneâ€“water systems. Journal of Chemical Physics, 2003, 119, 12417-12431.	1.2	136
28	Bulk Liquid Water at Ambient Temperature and Pressure from MP2 Theory. Journal of Physical Chemistry Letters, 2013, 4, 3753-3759.	2.1	131
29	Simulating Fluid-Phase Equilibria of Water from First Principlesâ€. Journal of Physical Chemistry A, 2006, 110, 640-646.	1.1	128
30	Carâ€“Parrinello molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 604-612.	6.2	128
31	Second-Order MÃ¸llerâ€“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, 4177-4188.	2.3	124
32	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, 2654-2671.	2.3	113
33	Thermal Effects on CH₃NH₃PbI₃ Perovskite from Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2015, 119, 8991-8997.	1.5	112
34	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, 1177-1182.	1.0	110
35	Car-Parrinello Molecular Dynamics on Massively Parallel Computers. ChemPhysChem, 2005, 6, 1788-1793.	1.0	105
36	Toward GW Calculations on Thousands of Atoms. Journal of Physical Chemistry Letters, 2018, 9, 306-312.	2.1	104

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37	Protonation-Dependent Binding of Ruthenium Bipyridyl Complexes to the Anatase(101) Surface. Journal of Physical Chemistry C, 2010, 114, 8398-8404.	1.5	103
38	Coverage Effect of the CO₂ Adsorption Mechanisms on CeO₂(111) by First Principles Analysis. Journal of Physical Chemistry C, 2013, 117, 1701-1711.	1.5	103
39	Ab initio molecular dynamics simulation of methanol adsorbed in chabazite. Chemical Physics Letters, 1997, 266, 397-402.	1.2	100
40	Isobaric-Isothermal Monte Carlo Simulations from First Principles: Application to Liquid Water at Ambient Conditions. ChemPhysChem, 2005, 6, 1894-1901.	1.0	99
41	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.	6.6	97
42	GW in the Gaussian and Plane Waves Scheme with Application to Linear Acenes. Journal of Chemical Theory and Computation, 2016, 12, 3623-3635.	2.3	97
43	Hexagonal boron nitride on transition metal surfaces. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	93
44	Structure and bonding in cisplatin and other Pt(II) complexes. Chemical Physics Letters, 1995, 234, 50-56.	1.2	91
45	Solvent effects on electronic properties from Wannier functions in a dimethyl sulfoxide/water mixture. Journal of Chemical Physics, 2004, 121, 5133-5142.	1.2	89
46	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, 4830-4833.	3.3	89
47	Real-World Predictions from Ab Initio Molecular Dynamics Simulations. Topics in Current Chemistry, 2011, 307, 109-153.	4.0	89
48	Probing the structural and dynamical properties of liquid water with models including non-local electron correlation. Journal of Chemical Physics, 2015, 143, 054506.	1.2	89
49	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.	6.6	87
50	Structural and Electronic Properties of Co-corrole, Co-corrin, and Co-porphyrin. Inorganic Chemistry, 2001, 40, 11-17.	1.9	84
51	Density functional embedding for molecular systems. Chemical Physics Letters, 2006, 421, 16-20.	1.2	84
52	Inner-shell spectroscopy by the Gaussian and augmented plane wave method. Physical Chemistry Chemical Physics, 2007, 9, 1599.	1.3	82
53	Control of Molecular Organization and Energy Level Alignment by an Electronically Nanopatterned Boron Nitride Template. ACS Nano, 2014, 8, 430-442.	7.3	75
54	A comparative study of O2, CO, and NO binding to iron-porphyrin. International Journal of Quantum Chemistry, 1998, 69, 31-35.	1.0	71

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55	A QM/MM Investigation of Thymine Dimer Radical Anion Splitting Catalyzed by DNA Photolyase. ChemPhysChem, 2009, 10, 400-410.	1.0	70
56	Microsolvation and Chemical Reactivity of Sodium and Water Clusters. Journal of the American Chemical Society, 2000, 122, 4837-4838.	6.6	66
57	Carâ€“Parrinello Molecular Dynamics Simulations of CaCl₂ Aqueous Solutions. Journal of Chemical Theory and Computation, 2008, 4, 779-789.	2.3	66
58	Nanotexture Switching of Singleâ€Layer Hexagonal Boron Nitride on Rhodium by Intercalation of Hydrogen Atoms. Angewandte Chemie - International Edition, 2010, 49, 6120-6124.	7.2	65
59	Simulation of Adsorption Processes at Metallic Interfaces: An Image Charge Augmented QM/MM Approach. Journal of Chemical Theory and Computation, 2013, 9, 5086-5097.	2.3	65
60	Towards a Rational Design of Ruthenium CO2 Hydrogenation Catalysts by Ab Initio Metadynamics. Chemistry - A European Journal, 2007, 13, 6828-6840.	1.7	63
61	Computational Study of Thymine Dimer Radical Anion Splitting in the Self-Repair Process of Duplex DNA. Journal of the American Chemical Society, 2008, 130, 3443-3450.	6.6	63
62	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, 2696-2701.	2.1	63
63	Endocyclic Cleavage in Glycosides with 2,3-transCyclic Protecting Groups. Journal of the American Chemical Society, 2011, 133, 5610-5619.	6.6	62
64	Classical polarizable force fields parametrized from ab initio calculations. Journal of Chemical Physics, 2002, 117, 1416-1433.	1.2	61
65	The structure of a DMSOâ€“water mixture from Carâ€“Parrinello simulations. Chemical Physics Letters, 2002, 364, 497-502.	1.2	61
66	Raman spectra from ab initio molecular dynamics and its application to liquid S-methyloxirane. Journal of Chemical Physics, 2014, 141, 094503.	1.2	61
67	Large-Scale Cubic-Scaling Random Phase Approximation Correlation Energy Calculations Using a Gaussian Basis. Journal of Chemical Theory and Computation, 2016, 12, 5851-5859.	2.3	61
68	Dual-level parallelism for ab initio molecular dynamics: Reaching teraflop performance with the CPMD code. Parallel Computing, 2005, 31, 1-17.	1.3	59
69	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.	0.8	59
70	Ab initio analysis of proton transfer dynamics in (H2O)3H+. Chemical Physics Letters, 2000, 321, 225-230.	1.2	54
71	Hartreeâ€“Fock exchange in time dependent density functional theory: application to charge transfer excitations in solvated molecular systems. Chemical Physics Letters, 2004, 394, 141-146.	1.2	54
72	Integrating the Carâ€“Parrinello equations. III. Techniques for ultrasoft pseudopotentials. Journal of Chemical Physics, 1995, 102, 859-871.	1.2	53

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73	Coupling of Surface Chemistry and Electric Double Layer at TiO₂ Electrochemical Interfaces. Journal of Physical Chemistry Letters, 2019, 10, 3871-3876.	2.1	53
74	Direct energy functional minimization under orthogonality constraints. Journal of Chemical Physics, 2008, 128, 084113.	1.2	52
75	Forces and stress in second order MÃ¸ller-Plesset perturbation theory for condensed phase systems within the resolution-of-identity Gaussian and plane waves approach. Journal of Chemical Physics, 2015, 143, 102803.	1.2	52
76	On the emergence of molecular structure. Physical Review A, 2011, 83, .	1.0	49
77	Computational Approaches to Activity in Rhodium-Catalysed Hydroformylation. Chemistry - A European Journal, 2004, 10, 2435-2444.	1.7	48
78	A Photochemical Activation Scheme of Inert Dinitrogen by Dinuclear RuII and FeII Complexes. Chemistry - A European Journal, 2004, 10, 4443-4453.	1.7	48
79	Magnetic linear response properties calculations with the Gaussian and augmented-plane-wave method. Journal of Chemical Physics, 2009, 131, 014106.	1.2	47
80	Accurate Hartree-Fock energy of extended systems using large Gaussian basis sets. Physical Review B, 2009, 80, .	1.1	47
81	Site-selective adsorption of phthalocyanine on h-BN/Rh(111) nanomesh. Physical Chemistry Chemical Physics, 2014, 16, 12374-12384.	1.3	47
82	Nonempirical Calculations of a Hydrated RNA Duplex. Journal of the American Chemical Society, 1996, 118, 8710-8712.	6.6	46
83	The molecular structure of C6: A theoretical investigation. Journal of Chemical Physics, 1994, 101, 2213-2216.	1.2	44
84	Dehalogenation and Coupling of a Polycyclic Hydrocarbon on an Atomically Thin Insulator. ACS Nano, 2014, 8, 6571-6579.	7.3	44
85	Mass density fluctuations in quantum and classical descriptions of liquid water. Journal of Chemical Physics, 2017, 146, 244501.	1.2	44
86	Notes on â€œEwald summation of electrostatic multipole interactions up to quadrupolar levelâ€•[J. Chem. Phys. 119, 7471 (2003)]. Journal of Chemical Physics, 2008, 129, 074102.	1.2	43
87	Investigation of Boron Nitride Nanomesh Interacting with Water. Journal of Physical Chemistry C, 2011, 115, 13685-13692.	1.5	43
88	Extracting elements of molecular structure from the all-particle wave function. Journal of Chemical Physics, 2011, 135, 204302.	1.2	43
89	Nonlocal van der Waals functionals: The case of rare-gas dimers and solids. Journal of Chemical Physics, 2013, 138, 204103.	1.2	42
90	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, 14307-14316.	1.3	42

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91	Enabling simulation at the fifth rung of DFT: Large scale RPA calculations with excellent time to solution. Computer Physics Communications, 2015, 187, 120-129.	3.0	42
92	Ground and Excited State Density Functional Calculations with the Gaussian and Augmented-Plane-Wave Method. Chimia, 2005, 59, 499-503.	0.3	41
93	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.	15.6	41
94	MoirÃ© beatings in graphene on Ru(0001). Physical Review B, 2013, 88, .	1.1	38
95	Quantifying the hydration structure of sodium and potassium ions: taking additional steps on Jacob's Ladder. Physical Chemistry Chemical Physics, 2020, 22, 10641-10652.	1.3	38
96	Modelling electrochemical systems with finite field molecular dynamics. JPhys Energy, 2020, 2, 032005.	2.3	38
97	Computational Investigation and Design of Cobalt Aqua Complexes for Homogeneous Water Oxidation. Journal of Physical Chemistry C, 2016, 120, 7966-7975.	1.5	37
98	Exploring the Limitation of Molecular Water Oxidation Catalysts. Journal of Physical Chemistry C, 2018, 122, 12404-12412.	1.5	37
99	Exponential transformation of molecular orbitals. Journal of Chemical Physics, 1994, 101, 3862-3865.	1.2	35
100	First-Principles Simulations of an Aqueous CO/Pt(111) Interface. Journal of Physical Chemistry C, 2018, 122, 24068-24076.	1.5	35
101	Nanoâ€ice on Boron Nitride Nanomesh: Accessing Proton Disorder. ChemPhysChem, 2010, 11, 399-403.	1.0	34
102	Structural and electronic properties of a large-scale MoirÃ© pattern of hexagonal boron nitride on Cu(111) studied with density functional theory. Nanoscale, 2013, 5, 5589.	2.8	34
103	Large-Scale Computation of Nuclear Magnetic Resonance Shifts for Paramagnetic Solids Using CP2K. Journal of Chemical Theory and Computation, 2018, 14, 377-394.	2.3	34
104	The molecular and electronic structure ofsâ€tetrazine in the ground and first excited state: A theoretical investigation. Journal of Chemical Physics, 1995, 103, 7048-7057.	1.2	33
105	s-Tetrazine in Aqueous Solution:Â A Density Functional Study of Hydrogen Bonding and Electronic Excitations. Journal of Physical Chemistry A, 2004, 108, 2044-2052.	1.1	33
106	CPMD: Car-Parrinello molecular dynamics. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.4	33
107	Dividing a complex reaction involving a hypervalent iodine reagent into three limiting mechanisms by ab initio molecular dynamics. Journal of Computational Chemistry, 2015, 36, 785-794.	1.5	32
108	Periodic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m calculations in the Gaussian and plane-waves scheme. Physical Review B, 2017, 95, .	1.1	32

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109	Car-Parrinello Molecular Dynamics Study of the Initial Dinitrogen Reduction Step in Sellmann-Type Nitrogenase Model Complexes. Chemistry - A European Journal, 2005, 11, 574-583.	1.7	31
110	Ionic Liquids from Carâ˜Parrinello Simulations, Part I:Â Liquid AlCl3. Journal of Physical Chemistry B, 2006, 110, 11475-11480.	1.2	31
111	Functionalization of CeO₂(1â€‰1â€‰1) by Deposition of Small Ni Clusters: Effects on CO₂ Adsorption and O Vacancy Formation. ChemCatChem, 2015, 7, 625-634.	1.8	31
112	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, 590-596.	1.2	30
113	HYDROPHOBIC HYDRATION FROM CARâ€“PARRINELLO SIMULATIONS. International Journal of Modern Physics B, 2004, 18, 1951-1962.	1.0	29
114	Toward a Monte Carlo program for simulating vaporâ€“liquid phase equilibria from first principles. Computer Physics Communications, 2005, 169, 289-294.	3.0	29
115	Synthesis and hydrogen adsorption properties of internally polarized 2,6-azulenedicarboxylate based metalâ€“organic frameworks. Journal of Materials Chemistry A, 2014, 2, 18823-18830.	5.2	29
116	From porphyrins to pyrphyrins: adsorption study and metalation of a molecular catalyst on Au(111). Nanoscale, 2016, 8, 7958-7968.	2.8	29
117	Carboplatin versus cisplatin: density functional approach to their molecular properties. Chemical Physics Letters, 1995, 246, 469-474.	1.2	28
118	Response Function Basis Sets:â€‰ Application to Density Functional Calculations. The Journal of Physical Chemistry, 1996, 100, 6231-6235.	2.9	28
119	Beyond Isotropic Tumbling Models: Nuclear Spin Relaxation in Liquids from First Principles. ChemPhysChem, 2008, 9, 2313-2316.	1.0	28
120	A Scheme for the Evaluation of Electron Delocalization and Conjugation Efficiency in Linearly Ï€-Conjugated Systems. Journal of Chemical Theory and Computation, 2009, 5, 506-514.	2.3	28
121	Efficient Linear-Scaling Density Functional Theory for Molecular Systems. Journal of Chemical Theory and Computation, 2013, 9, 4421-4427.	2.3	28
122	A First Principles Investigation of the Structure of a Bacteriochlorophyll Crystal. Journal of the American Chemical Society, 1996, 118, 7847-7848.	6.6	25
123	Lowâ€Barrier Pathway for endoâ€Cleavage Induced Anomerization of Pyranosides with Nâ€Benzylâ€2,3â€transâ€oxazolidinone Groups. European Journal of Organic Chemistry, 2009, 2009, 1127-1131.	1.2	23
124	Liquid Water through Density-Functional Molecular Dynamics: Plane-Wave vs Atomic-Orbital Basis Sets. Journal of Chemical Theory and Computation, 2016, 12, 3456-3462.	2.3	23
125	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.	6.6	22
126	Semiempirical Self-Consistent Polarization Description of Bulk Water, the Liquidâ˜Vapor Interface, and Cubic Ice. Journal of Physical Chemistry A, 2011, 115, 6046-6053.	1.1	22

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127	Non-innocent adsorption of Co-pyrphyrin on rutile(110). Physical Chemistry Chemical Physics, 2015, 17, 22846-22854.	1.3	22
128	Excited state geometries within time-dependent and restricted open-shell density functional theories. Computational and Theoretical Chemistry, 2003, 630, 163-175.	1.5	21
129	Significant Substituent Effect on the Anomerization of Pyranosides: Mechanism of Anomerization and Synthesis of a 1,2â€‹cis Glucosamine Oligomer from the 1,2â€‹trans Anomer. Chemistry - A European Journal, 2014, 20, 124-132.	1.7	21
130	Polarized atomic orbitals for linear scaling methods. Journal of Chemical Physics, 2002, 116, 1800-1810.	1.2	20
131	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.	0.7	19
132	C61H2 in Molecular and Solid Phases: Density-Functional Approach to Structural and Electronic Properties. The Journal of Physical Chemistry, 1995, 99, 4008-4014.	2.9	18
133	Towards electronic structure-based ab-initio molecular dynamics simulations with hundreds of millions of atoms. Parallel Computing, 2022, 111, 102920.	1.3	17
134	Correction to â€œBulk Liquid Water at Ambient Temperature and Pressure from MP2 Theoryâ€• Journal of Physical Chemistry Letters, 2014, 5, 3066-3067.	2.1	16
135	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.	1.5	16
136	A density-functional approach to polarizable models: A Kim-Gordon response density interaction potential for molecular simulations. Journal of Chemical Physics, 2005, 123, 074108.	1.2	14
137	A smooth â„“1-norm sparseness function for orbital based linear scaling total energy minimization. Journal of Chemical Physics, 2008, 128, 064107.	1.2	14
138	Double-Hybrid DFT Functionals for the Condensed Phase: Gaussian and Plane Waves Implementation and Evaluation. Molecules, 2020, 25, 5174.	1.7	14
139	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.	1.3	14
140	Building Blocks for Two-Dimensional Metalâ€“Organic Frameworks Confined at the Airâ€“Water Interface: An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry C, 2015, 119, 4023-4030.	1.5	13
141	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.	1.2	12
142	Excited-State Properties for Extended Systems: Efficient Hybrid Density Functional Methods. Journal of Chemical Theory and Computation, 2022, 18, 4186-4202.	2.3	12
143	The structure ofn-fold negatively charged C60(n= 1, 2,â€¦,6). International Journal of Quantum Chemistry, 1993, 46, 81-86.	1.0	10
144	Chiral Distortion of Confined Ice Oligomers (n = 5,6). Langmuir, 2012, 28, 15246-15250.	1.6	10

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145	Impact of Donorâ€“Acceptor Functionalization on the Properties of Linearly Ï€-Conjugated Oligomers: Establishing Quantitative Relationships for the Substituent and Substituent Cooperative Effect Based on Quantum Chemical Calculations. Journal of Organic Chemistry, 2013, 78, 12681-12689.	1.7	10
146	Local Fitting of the Kohnâ€“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.	2.3	10
147	Mapping the Free Energy of Lithium Solvation in the Protic Ionic Liquid Ethylammonuim Nitrate: A Metadynamics Study. ChemSusChem, 2017, 10, 3083-3090.	3.6	10
148	Comment on â€œDissociation of Water under Pressureâ€. Physical Review Letters, 2002, 89, 199601; author reply 199602.	2.9	9
149	Chemical Reactions on Metal-supported Hexagonal Boron Nitride Investigated with Density Functional Theory. Chimia, 2014, 68, 596.	0.3	9
150	Investigation of h -BN/Rh(111) Nanomesh Interacting with Water and Atomic Hydrogen. Chimia, 2011, 65, 256.	0.3	8
151	Describing the chemical bonding in C70 and C70O3 â€“ A quantum chemical topology study. Chemical Physics, 2014, 433, 22-30.	0.9	8
152	Increasing the Efficiency of Sparse Matrix-Matrix Multiplication with a 2.5D Algorithm and One-Sided MPI. , 2017, , .		8
153	The impact of metalation on adsorption geometry, electronic level alignment and UV-stability of organic macrocycles on TiO₂(110). Nanoscale, 2017, 9, 8756-8763.	2.8	7
154	Second generation Car-Parrinello MD: application to the h-BN/Rh(111) nanomesh. European Physical Journal B, 2018, 91, 1.	0.6	7
155	First-principles correction scheme for linear-response time-dependent density functional theory calculations of core electronic states. Journal of Chemical Physics, 2021, 155, 034108.	1.2	7
156	Double-hybrid density functionals for the condensed phase: Gradients, stress tensor, and auxiliary-density matrix method acceleration. Journal of Chemical Physics, 2022, 156, 074107.	1.2	7
157	Local Disorder in Lithium Imide from Density Functional Simulation and NMR Spectroscopy. Journal of Physical Chemistry C, 2012, 116, 18577-18583.	1.5	6
158	Postâ€Synthesis Amine Borane Functionalization of a Metalâ€Organic Framework and Its Unusual Chemical Hydrogen Release Phenomenon. Chemistry - A European Journal, 2017, 23, 8823-8828.	1.7	6
159	Formation and properties of a terpyridine-based 2D MOF on the surface of water. 2D Materials, 2016, 3, 025026.	2.0	5
160	Nano-ice models for the water aggregates observed on the h-BN/Rh(111) nanomesh. Journal of Physics Condensed Matter, 2012, 24, 445002.	0.7	3
161	Time and Length Scales in ab initio Molecular Dynamics. Lecture Notes in Physics, 2002, , 413-442.	0.3	3
162	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.	1.2	2

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163	MP2- and RPA-Based Ab Initio Molecular Dynamics and Monte Carlo Sampling. , 2018, , 1-21.		1
164	DBCSR: A Library for Dense Matrix Multiplications on Distributed GPU-Accelerated Systems. , 2019, , .		1
165	DBCSR: A Blocked Sparse Tensor Algebra Library. Advances in Parallel Computing, 2020, , .	0.3	1
166	MP2- and RPA-Based Ab Initio Molecular Dynamics and Monte Carlo Sampling. , 2020, , 523-543.		0