Joost VandeVondele

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2827070/publications.pdf

Version: 2024-02-01

111 papers	19,224 citations	38660 50 h-index	28224 105 g-index
116 all docs	116 docs citations	116 times ranked	13791 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	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
5	Catalyst support effects on hydrogen spillover. Nature, 2017, 541, 68-71.	13.7	639
6	A Hamiltonian electrostatic coupling scheme for hybrid Carâ€“Parrinello molecular dynamics simulations. Journal of Chemical Physics, 2002, 116, 6941-6947.	1.2	588
7	An efficient orbital transformation method for electronic structure calculations. Journal of Chemical Physics, 2003, 118, 4365-4369.	1.2	460
8	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
9	Auxiliary Density Matrix Methods for Hartreeâ^'Fock Exchange Calculations. Journal of Chemical Theory and Computation, 2010, 6, 2348-2364.	2.3	438
10	Liquid Water from First Principles:Â Investigation of Different Sampling Approaches. Journal of Physical Chemistry B, 2004, 108, 12990-12998.	1.2	327
11	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
12	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
13	Ab initio molecular dynamics using hybrid density functionals. Journal of Chemical Physics, 2008, 128, 214104.	1.2	207
14	Materials Cloud, a platform for open computational science. Scientific Data, 2020, 7, 299.	2.4	189
15	D-RESP:â€‰ Dynamically Generated Electrostatic Potential Derived Charges from Quantum Mechanics/Molecular Mechanics Simulations. Journal of Physical Chemistry B, 2002, 106, 7300-7307.	1.2	187
16	Redox Potentials and Acidity Constants from Density Functional Theory Based Molecular Dynamics. Accounts of Chemical Research, 2014, 47, 3522-3529.	7.6	181
17	A molecular dynamics study of the hydroxyl radical in solution applying self-interaction-corrected density functional methods. Physical Chemistry Chemical Physics, 2005, 7, 1363.	1.3	159
18	Synthesis of a Covalent Monolayer Sheet by Photochemical Anthracene Dimerization at the Air/Water Interface and its Mechanical Characterization by AFM Indentation. Advanced Materials, 2014, 26, 2052-2058.	11.1	147

#	Article	IF	Citations
19	Sparse matrix multiplication: The distributed block-compressed sparse row library. Parallel Computing, 2014, 40, 47-58.	1.3	143
20	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
21	Bulk Liquid Water at Ambient Temperature and Pressure from MP2 Theory. Journal of Physical Chemistry Letters, 2013, 4, 3753-3759.	2.1	131
22	Simulating Fluid-Phase Equilibria of Water from First Principlesâ€. Journal of Physical Chemistry A, 2006, 110, 640-646.	1.1	128
23	Synthesis of Two-Dimensional Analogues of Copolymers by Site-to-Site Transmetalation of Organometallic Monolayer Sheets. Journal of the American Chemical Society, 2014, 136, 6103-6110.	6.6	128
24	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
25	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
26	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
27	Protonation-Dependent Binding of Ruthenium Bipyridyl Complexes to the Anatase(101) Surface. Journal of Physical Chemistry C, 2010, 114, 8398-8404.	1.5	103
28	Isobaric-Isothermal Monte Carlo Simulations from First Principles: Application to Liquid Water at Ambient Conditions. ChemPhysChem, 2005, 6, 1894-1901.	1.0	99
29	Structure, Dynamics, and Reactivity of Hydrated Electrons by Ab Initio Molecular Dynamics. Accounts of Chemical Research, 2012, 45, 23-32.	7.6	98
30	The nature of excess electrons in anatase and rutile from hybrid DFT and RPA. Physical Chemistry Chemical Physics, 2014, 16, 26144-26152.	1.3	95
31	Polarization- and Azimuth-Resolved Infrared Spectroscopy of Water on TiO₂(110): Anisotropy and the Hydrogen-Bonding Network. Journal of Physical Chemistry Letters, 2012, 3, 778-784.	2.1	91
32	Chasing charge localization and chemical reactivity following photoionization in liquid water. Journal of Chemical Physics, 2011, 135, 224510.	1.2	90
33	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
34	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
35	Calculation of Redox Properties:â€‰ Understanding Short- and Long-Range Effects in Rubredoxin. Journal of Physical Chemistry B, 2007, 111, 3969-3976.	1.2	88
36	Identifying Trapped Electronic Holes at the Aqueous TiO₂ Interface. Journal of Physical Chemistry C, 2014, 118, 5437-5444.	1.5	85

#	Article	IF	Citations
37	Electronic Structure of the Water Dimer Cation. Journal of Physical Chemistry A, 2008, 112, 6159-6170.	1.1	84
38	Ab Initio Molecular Dynamics Simulation of a Medium-Sized Water Cluster Anion: From an Interior to a Surface-Located Excess Electron via a Delocalized State. Journal of Physical Chemistry A, 2008, 112, 6125-6133.	1.1	79
39	Aqueous Redox Chemistry and the Electronic Band Structure of Liquid Water. Journal of Physical Chemistry Letters, 2012, 3, 3411-3415.	2.1	76
40	Aligning Electronic and Protonic Energy Levels of Protonâ€Coupled Electron Transfer in Water Oxidation on Aqueous TiO₂. Angewandte Chemie - International Edition, 2014, 53, 12046-12050.	7.2	74
41	Canonical Adiabatic Free Energy Sampling (CAFES):â€‰ A Novel Method for the Exploration of Free Energy Surfaces. Journal of Physical Chemistry B, 2002, 106, 203-208.	1.2	70
42	Molecular Ordering at the Interface Between Liquid Water and Rutile TiO₂(110). Advanced Materials Interfaces, 2015, 2, 1500246.	1.9	68
43	Hole Localization and Thermochemistry of Oxidative Dehydrogenation of Aqueous Rutile TiO₂(110). ChemCatChem, 2012, 4, 636-640.	1.8	65
44	Hybrid QM/MM Car-Parrinello Simulations of Catalytic and Enzymatic Reactions. Chimia, 2002, 56, 13-19.	0.3	62
45	Large variation of vacancy formation energies in the surface of crystalline ice. Nature Materials, 2011, 10, 794-798.	13.3	59
46	Combining Linear-Scaling DFT with Subsystem DFT in Bornâ€“Oppenheimer and Ehrenfest Molecular Dynamics Simulations: From Molecules to a Virus in Solution. Journal of Chemical Theory and Computation, 2016, 12, 3214-3227.	2.3	59
47	Accurate molecular dynamics and nuclear quantum effects at low cost by multiple steps in real and imaginary time: Using density functional theory to accelerate wavefunction methods. Journal of Chemical Physics, 2016, 144, 054111.	1.2	58
48	Dynamics of the Bulk Hydrated Electron from Manyâ€Body Waveâ€Function Theory. Angewandte Chemie - International Edition, 2019, 58, 3890-3893.	7.2	53
49	Direct energy functional minimization under orthogonality constraints. Journal of Chemical Physics, 2008, 128, 084113.	1.2	52
50	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
51	Red-blue pebbling revisited. , 2019, , .		50
52	Periodic MP2, RPA, and Boundary Condition Assessment of Hydrogen Ordering in Ice XV. Journal of Physical Chemistry Letters, 2014, 5, 4122-4128.	2.1	48
53	Reaction mechanism of caspases: Insights from QM/MM Car-Parrinello simulations. Proteins: Structure, Function and Bioinformatics, 2003, 52, 212-224.	1.5	47
54	The Electron Attachment Energy of the Aqueous Hydroxyl Radical Predicted from the Detachment Energy of the Aqueous Hydroxide Anion. Journal of the American Chemical Society, 2009, 131, 6046-6047.	6.6	47

#	Article	IF	Citations
55	Accurate Hartree-Fock energy of extended systems using large Gaussian basis sets. Physical Review B, 2009, 80, .	1.1	47
56	Effect of Counter Ions on the Silica Oligomerization Reaction. ChemPhysChem, 2009, 10, 1775-1782.	1.0	46
57	Characterization of the Dizinc Analogue of the Synthetic Diiron Protein DF1 Using ab Initio and Hybrid Quantum/Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2003, 107, 4182-4188.	1.2	43
58	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
59	Vibrational Spectra of Phosphate Ions in Aqueous Solution Probed by First-Principles Molecular Dynamics. Journal of Physical Chemistry A, 2012, 116, 2466-2474.	1.1	41
60	A Variational Definition of Electrostatic Potential Derived Charges. Journal of Physical Chemistry B, 2004, 108, 7963-7968.	1.2	40
61	Density Functional Theory Study of Tetrathiafulvalene and Thianthrene in Acetonitrile:Â Structure, Dynamics, and Redox Propertiesâ€. Journal of Physical Chemistry B, 2006, 110, 3614-3623.	1.2	38
62	Calculation of Electrochemical Energy Levels in Water Using the Random Phase Approximation and a Double Hybrid Functional. Physical Review Letters, 2016, 116, 086402.	2.9	38
63	Decisive Role of Perimeter Sites in Silica-Supported Ag Nanoparticles in Selective Hydrogenation of CO₂ to Methyl Formate in the Presence of Methanol. Journal of the American Chemical Society, 2018, 140, 13884-13891.	6.6	37
64	Redox free energies and one-electron energy levels in density functional theory based ab initio molecular dynamics. Journal of Electroanalytical Chemistry, 2007, 607, 113-120.	1.9	36
65	Hydrogen Adsorption on Nanosized Platinum and Dynamics of Spillover onto Alumina and Titania. Journal of Physical Chemistry C, 2017, 121, 17862-17872.	1.5	36
66	Machine Learning Adaptive Basis Sets for Efficient Large Scale Density Functional Theory Simulation. Journal of Chemical Theory and Computation, 2018, 14, 4168-4175.	2.3	36
67	Importance of the Number of Acid Molecules and the Strength of the Base for Double-Ion Formation in (H₂SO₄)_mÂ·BaseÂ·(H₂O)₆ Clusters. Journal of the American Chemical Society, 2008, 130, 14144-14147.	6.6	34
68	Hydrogen Forms in Water by Proton Transfer to a Distorted Electron. Journal of Physical Chemistry B, 2010, 114, 915-920.	1.2	33
69	Point defects at the ice (0001) surface. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 12429-12434.	3.3	32
70	Efficient multidimensional free energy calculations for ab initio molecular dynamics using classical bias potentials. Journal of Chemical Physics, 2000, 113, 4863.	1.2	30
71	A Consistent Picture of the Proton Release Mechanism of oNBA in Water by Ultrafast Spectroscopy and Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2011, 115, 1075-1083.	1.2	30
72	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

#	Article	IF	Citations
73	First-principles molecular dynamics of metallic systems. Physical Review B, 1999, 60, 13241-13244.	1.1	29
74	Toward a Monte Carlo program for simulating vaporâ€“liquid phase equilibria from first principles. Computer Physics Communications, 2005, 169, 289-294.	3.0	29
75	From Solvent Fluctuations to Quantitative Redox Properties of Quinones in Methanol and Acetonitrile. Angewandte Chemie - International Edition, 2006, 45, 1936-1938.	7.2	29
76	Efficient Linear-Scaling Density Functional Theory for Molecular Systems. Journal of Chemical Theory and Computation, 2013, 9, 4421-4427.	2.3	28
77	Spin-Unrestricted Second-Order MÃ¸llerâ€“Plesset (MP2) Forces for the Condensed Phase: From Molecular Radicals to F-Centers in Solids. Journal of Chemical Theory and Computation, 2016, 12, 2214-2223.	2.3	25
78	Copper binding sites in the Câ€terminal domain of mouse prion protein: A hybrid (QM/MM) molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1084-1098.	1.5	21
79	Accelerating Rare Reactive Events by Means of a Finite Electronic Temperature. Journal of the American Chemical Society, 2002, 124, 8163-8171.	6.6	20
80	Reductive Hydrogenation of the Aqueous Rutile TiO 2 (110) Surface. Electrochimica Acta, 2015, 179, 658-667.	2.6	20
81	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
82	Structure and Mobility of Acetic Acid at the Anatase (101)/Acetonitrile Interface. Journal of Physical Chemistry C, 2014, 118, 6251-6260.	1.5	19
83	A generalized Poisson solver for first-principles device simulations. Journal of Chemical Physics, 2016, 144, 044113.	1.2	18
84	Efficient algorithms for large-scale quantum transport calculations. Journal of Chemical Physics, 2017, 147, 074116.	1.2	18
85	Role of Water, CO₂, and Noninnocent Ligands in the CO₂ Hydrogenation to Formate by an Ir(III) PNP Pincer Catalyst Evaluated by Static-DFT and ab Initio Molecular Dynamics under Reaction Conditions. Organometallics, 2017, 36, 4908-4919.	1.1	18
86	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
87	Pushing back the limit of ab-initio quantum transport simulations on hybrid supercomputers. , 2015, , .		16
88	First-Principles Monte Carlo Simulations of Reaction Equilibria in Compressed Vapors. ACS Central Science, 2016, 2, 409-415.	5.3	16
89	Ab initiomolecular dynamics study of ascorbic acid in aqueous solution. Molecular Physics, 2007, 105, 17-23.	0.8	14
90	Excess Electrons and Interstitial Li Atoms in TiO₂ Anatase: Properties of the (101) Interface. Journal of Physical Chemistry C, 2015, 119, 15009-15018.	1.5	14

#	Article	IF	Citations
91	Three- and Four-Center Trans Effects in Triply Bonded Ditungsten Complexes:Â An ab Initio Molecular Dynamics Study of Compounds with Stoichiometry W2Cl4(NHEt)2(PMe3)2. Inorganic Chemistry, 2000, 39, 5553-5560.	1.9	12
92	Speed Limits for Acidâ€“Base Chemistry in Aqueous Solutions. Chimia, 2012, 66, 182-186.	0.3	12
93	Solvation of p-Coumaric Acid in Water. Journal of Physical Chemistry B, 2007, 111, 13591-13599.	1.2	10
94	Nuclear Quantum Effects on Aqueous Electron Attachment and Redox Properties. Journal of Physical Chemistry Letters, 2017, 8, 1424-1428.	2.1	10
95	A comparison of accelerators for direct energy minimization in electronic structure calculations. Journal of Chemical Physics, 2011, 134, 244104.	1.2	9
96	GridTools: A framework for portable weather and climate applications. SoftwareX, 2021, 15, 100707.	1.2	9
97	Cisâ^'TransIsomerization in Triply-Bonded Ditungsten Complexes:Â A Multitude of Possible Pathways. Inorganic Chemistry, 2001, 40, 5780-5786.	1.9	8
98	Large Scale Condensed Matter Calculations using the Gaussian and Augmented Plane Waves Method. , 2006, , 287-314.		8
99	Insight into Fundamental, Overtone, and Combination IR Bands of Surface and Bulk Ba(NO₃)₂ by Ab Initio Molecular Dynamics. Journal of Physical Chemistry C, 2010, 114, 15042-15048.	1.5	8
100	Increasing the Efficiency of Sparse Matrix-Matrix Multiplication with a 2.5D Algorithm and One-Sided MPI. , 2017, , .		8
101	Large scale simulation of pressure induced phase-field fracture propagation using Utopia. CCF Transactions on High Performance Computing, 2021, 3, 407-426.	1.1	7
102	On the parallel I/O optimality of linear algebra kernels. , 2021, , .		7
103	Electron Transfer Properties from Atomistic Simulations and Density Functional Theory. Chimia, 2007, 61, 155-158.	0.3	6
104	Efficient preconditioning of the electronic structure problem in large scale ab initio molecular dynamics simulations. Journal of Chemical Physics, 2015, 142, 244117.	1.2	6
105	Microcanonical RT-TDDFT simulations of realistically extended devices. Journal of Chemical Physics, 2018, 149, 124701.	1.2	4
106	Dynamics of the Bulk Hydrated Electron from Manyâ€Body Waveâ€Function Theory. Angewandte Chemie, 2019, 131, 3930-3933.	1.6	4
107	Estimating equilibrium properties from non-Hamiltonian dynamics. Journal of Chemical Physics, 2001, 115, 7859-7864.	1.2	2
108	Towards ab-initio simulations of nanowire field-effect transistors. , 2014, , .		2

#	Article	IF	Citations
109	Transport simulations with density-matrix-based real-time time-dependant density functional theory. , 2017, , .		1
110	MP2- and RPA-Based Ab Initio Molecular Dynamics and Monte Carlo Sampling. , 2018, , 1-21.		1
111	MP2- and RPA-Based Ab Initio Molecular Dynamics and Monte Carlo Sampling. , 2020, , 523-543.		0