

# Joost VandeVondele

## List of Publications by Year in descending order

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111  
papers

19,224  
citations

38742

50  
h-index

28297

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. <i>Computer Physics Communications</i> , 2005, 167, 103-128.	7.5	4,200
2	Gaussian basis sets for accurate calculations on molecular systems in gas and condensed phases. <i>Journal of Chemical Physics</i> , 2007, 127, 114105.	3.0	2,793
3	<scp>cp2k:</scp> atomistic simulations of condensed matter systems. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 15-25.	14.6	2,049
4	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. <i>Journal of Chemical Physics</i> , 2020, 152, 194103.	3.0	1,371
5	Catalyst support effects on hydrogen spillover. <i>Nature</i> , 2017, 541, 68-71.	27.8	639
6	A Hamiltonian electrostatic coupling scheme for hybrid Carâ€Parrinello molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2002, 116, 6941-6947.	3.0	588
7	An efficient orbital transformation method for electronic structure calculations. <i>Journal of Chemical Physics</i> , 2003, 118, 4365-4369.	3.0	460
8	The influence of temperature and density functional models in ab initio molecular dynamics simulation of liquid water. <i>Journal of Chemical Physics</i> , 2005, 122, 014515.	3.0	444
9	Auxiliary Density Matrix Methods for HartreeâˆFock Exchange Calculations. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2348-2364.	5.3	438
10	Liquid Water from First Principles:Â Investigation of Different Sampling Approaches. <i>Journal of Physical Chemistry B</i> , 2004, 108, 12990-12998.	2.6	327
11	IsobaricâˆIsothermal Molecular Dynamics Simulations Utilizing Density Functional Theory: An Assessment of the Structure and Density of Water at Near-Ambient Conditions. <i>Journal of Physical Chemistry B</i> , 2009, 113, 11959-11964.	2.6	327
12	Robust Periodic HartreeâˆFock Exchange for Large-Scale Simulations Using Gaussian Basis Sets. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 3010-3021.	5.3	254
13	<i>Ab initio</i> molecular dynamics using hybrid density functionals. <i>Journal of Chemical Physics</i> , 2008, 128, 214104.	3.0	207
14	Materials Cloud, a platform for open computational science. <i>Scientific Data</i> , 2020, 7, 299.	5.3	189
15	D-RESP:â€ Dynamically Generated Electrostatic Potential Derived Charges from Quantum Mechanics/Molecular Mechanics Simulations. <i>Journal of Physical Chemistry B</i> , 2002, 106, 7300-7307.	2.6	187
16	Redox Potentials and Acidity Constants from Density Functional Theory Based Molecular Dynamics. <i>Accounts of Chemical Research</i> , 2014, 47, 3522-3529.	15.6	181
17	A molecular dynamics study of the hydroxyl radical in solution applying self-interaction-corrected density functional methods. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 1363.	2.8	159
18	Synthesis of a Covalent Monolayer Sheet by Photochemical Anthracene Dimerization at the Air/Water Interface and its Mechanical Characterization by AFM Indentation. <i>Advanced Materials</i> , 2014, 26, 2052-2058.	21.0	147

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19	Sparse matrix multiplication: The distributed block-compressed sparse row library. <i>Parallel Computing</i> , 2014, 40, 47-58.	2.1	143
20	Linear Scaling Self-Consistent Field Calculations with Millions of Atoms in the Condensed Phase. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3565-3573.	5.3	138
21	Bulk Liquid Water at Ambient Temperature and Pressure from MP2 Theory. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 3753-3759.	4.6	131
22	Simulating Fluid-Phase Equilibria of Water from First Principles. <i>Journal of Physical Chemistry A</i> , 2006, 110, 640-646.	2.5	128
23	Synthesis of Two-Dimensional Analogues of Copolymers by Site-to-Site Transmetalation of Organometallic Monolayer Sheets. <i>Journal of the American Chemical Society</i> , 2014, 136, 6103-6110.	13.7	128
24	Second-Order Møller-Plesset Perturbation Theory in the Condensed Phase: An Efficient and Massively Parallel Gaussian and Plane Waves Approach. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4177-4188.	5.3	124
25	Electron Correlation in the Condensed Phase from a Resolution of Identity Approach Based on the Gaussian and Plane Waves Scheme. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2654-2671.	5.3	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. <i>ChemPhysChem</i> , 2003, 4, 1177-1182.	2.1	110
27	Protonation-Dependent Binding of Ruthenium Bipyridyl Complexes to the Anatase(101) Surface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 8398-8404.	3.1	103
28	Isobaric-Isothermal Monte Carlo Simulations from First Principles: Application to Liquid Water at Ambient Conditions. <i>ChemPhysChem</i> , 2005, 6, 1894-1901.	2.1	99
29	Structure, Dynamics, and Reactivity of Hydrated Electrons by Ab Initio Molecular Dynamics. <i>Accounts of Chemical Research</i> , 2012, 45, 23-32.	15.6	98
30	The nature of excess electrons in anatase and rutile from hybrid DFT and RPA. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26144-26152.	2.8	95
31	Polarization- and Azimuth-Resolved Infrared Spectroscopy of Water on TiO <sub>2</sub> (110): Anisotropy and the Hydrogen-Bonding Network. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 778-784.	4.6	91
32	Chasing charge localization and chemical reactivity following photoionization in liquid water. <i>Journal of Chemical Physics</i> , 2011, 135, 224510.	3.0	90
33	An atomistic picture of the regeneration process in dye sensitized solar cells. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 4830-4833.	7.1	89
34	Probing the structural and dynamical properties of liquid water with models including non-local electron correlation. <i>Journal of Chemical Physics</i> , 2015, 143, 054506.	3.0	89
35	Calculation of Redox Properties: Understanding Short- and Long-Range Effects in Rubredoxin. <i>Journal of Physical Chemistry B</i> , 2007, 111, 3969-3976.	2.6	88
36	Identifying Trapped Electronic Holes at the Aqueous TiO <sub>2</sub> Interface. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5437-5444.	3.1	85

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37	Electronic Structure of the Water Dimer Cation. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6159-6170.	2.5	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. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6125-6133.	2.5	79
39	Aqueous Redox Chemistry and the Electronic Band Structure of Liquid Water. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3411-3415.	4.6	76
40	Aligning Electronic and Protonic Energy Levels of Proton-Coupled Electron Transfer in Water Oxidation on Aqueous TiO <sub>2</sub> . <i>Angewandte Chemie - International Edition</i> , 2014, 53, 12046-12050.	13.8	74
41	Canonical Adiabatic Free Energy Sampling (CAFES): A Novel Method for the Exploration of Free Energy Surfaces. <i>Journal of Physical Chemistry B</i> , 2002, 106, 203-208.	2.6	70
42	Molecular Ordering at the Interface Between Liquid Water and Rutile TiO <sub>2</sub> (110). <i>Advanced Materials Interfaces</i> , 2015, 2, 1500246.	3.7	68
43	Hole Localization and Thermochemistry of Oxidative Dehydrogenation of Aqueous Rutile TiO <sub>2</sub> (110). <i>ChemCatChem</i> , 2012, 4, 636-640.	3.7	65
44	Hybrid QM/MM Car-Parrinello Simulations of Catalytic and Enzymatic Reactions. <i>Chimia</i> , 2002, 56, 13-19.	0.6	62
45	Large variation of vacancy formation energies in the surface of crystalline ice. <i>Nature Materials</i> , 2011, 10, 794-798.	27.5	59
46	Combining Linear-Scaling DFT with Subsystem DFT in Born-Oppenheimer and Ehrenfest Molecular Dynamics Simulations: From Molecules to a Virus in Solution. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3214-3227.	5.3	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. <i>Journal of Chemical Physics</i> , 2016, 144, 054111.	3.0	58
48	Dynamics of the Bulk Hydrated Electron from Many-Body Wavefunction Theory. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 3890-3893.	13.8	53
49	Direct energy functional minimization under orthogonality constraints. <i>Journal of Chemical Physics</i> , 2008, 128, 084113.	3.0	52
50	Forces and stress in second order Møller-Plesset perturbation theory for condensed phase systems within the resolution-of-identity Gaussian and plane waves approach. <i>Journal of Chemical Physics</i> , 2015, 143, 102803.	3.0	52
51	Red-blue pebbling revisited. , 2019, , .		50
52	Periodic MP2, RPA, and Boundary Condition Assessment of Hydrogen Ordering in Ice XV. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 4122-4128.	4.6	48
53	Reaction mechanism of caspases: Insights from QM/MM Car-Parrinello simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 52, 212-224.	2.6	47
54	The Electron Attachment Energy of the Aqueous Hydroxyl Radical Predicted from the Detachment Energy of the Aqueous Hydroxide Anion. <i>Journal of the American Chemical Society</i> , 2009, 131, 6046-6047.	13.7	47

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55	Accurate Hartree-Fock energy of extended systems using large Gaussian basis sets. <i>Physical Review B</i> , 2009, 80, .	3.2	47
56	Effect of Counter Ions on the Silica Oligomerization Reaction. <i>ChemPhysChem</i> , 2009, 10, 1775-1782.	2.1	46
57	Characterization of the Dizinc Analogue of the Synthetic Diiron Protein DF1 Using ab Initio and Hybrid Quantum/Classical Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2003, 107, 4182-4188.	2.6	43
58	Enabling simulation at the fifth rung of DFT: Large scale RPA calculations with excellent time to solution. <i>Computer Physics Communications</i> , 2015, 187, 120-129.	7.5	42
59	Vibrational Spectra of Phosphate Ions in Aqueous Solution Probed by First-Principles Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2466-2474.	2.5	41
60	A Variational Definition of Electrostatic Potential Derived Charges. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7963-7968.	2.6	40
61	Density Functional Theory Study of Tetrathiafulvalene and Thianthrene in Acetonitrile: Structure, Dynamics, and Redox Properties. <i>Journal of Physical Chemistry B</i> , 2006, 110, 3614-3623.	2.6	38
62	Calculation of Electrochemical Energy Levels in Water Using the Random Phase Approximation and a Double Hybrid Functional. <i>Physical Review Letters</i> , 2016, 116, 086402.	7.8	38
63	Decisive Role of Perimeter Sites in Silica-Supported Ag Nanoparticles in Selective Hydrogenation of CO <sub>2</sub> to Methyl Formate in the Presence of Methanol. <i>Journal of the American Chemical Society</i> , 2018, 140, 13884-13891.	13.7	37
64	Redox free energies and one-electron energy levels in density functional theory based ab initio molecular dynamics. <i>Journal of Electroanalytical Chemistry</i> , 2007, 607, 113-120.	3.8	36
65	Hydrogen Adsorption on Nanosized Platinum and Dynamics of Spillover onto Alumina and Titania. <i>Journal of Physical Chemistry C</i> , 2017, 121, 17862-17872.	3.1	36
66	Machine Learning Adaptive Basis Sets for Efficient Large Scale Density Functional Theory Simulation. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4168-4175.	5.3	36
67	Importance of the Number of Acid Molecules and the Strength of the Base for Double-Ion Formation in (H <sub>2</sub> SO <sub>4</sub> ) <sub>m</sub> ·Base·(H <sub>2</sub> O) <sub>6</sub> Clusters. <i>Journal of the American Chemical Society</i> , 2008, 130, 14144-14147.	13.7	34
68	Hydrogen Forms in Water by Proton Transfer to a Distorted Electron. <i>Journal of Physical Chemistry B</i> , 2010, 114, 915-920.	2.6	33
69	Point defects at the ice (0001) surface. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 12429-12434.	7.1	32
70	Efficient multidimensional free energy calculations for ab initio molecular dynamics using classical bias potentials. <i>Journal of Chemical Physics</i> , 2000, 113, 4863.	3.0	30
71	A Consistent Picture of the Proton Release Mechanism of <i>io</i> NBA in Water by Ultrafast Spectroscopy and Ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2011, 115, 1075-1083.	2.6	30
72	Dielectric Properties of Water Ice, the Ice Ih/XI Phase Transition, and an Assessment of Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2014, 118, 590-596.	2.6	30

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73	First-principles molecular dynamics of metallic systems. <i>Physical Review B</i> , 1999, 60, 13241-13244.	3.2	29
74	Toward a Monte Carlo program for simulating vapor-liquid phase equilibria from first principles. <i>Computer Physics Communications</i> , 2005, 169, 289-294.	7.5	29
75	From Solvent Fluctuations to Quantitative Redox Properties of Quinones in Methanol and Acetonitrile. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 1936-1938.	13.8	29
76	Efficient Linear-Scaling Density Functional Theory for Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4421-4427.	5.3	28
77	Spin-Unrestricted Second-Order Møller-Plesset (MP2) Forces for the Condensed Phase: From Molecular Radicals to F-Centers in Solids. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2214-2223.	5.3	25
78	Copper binding sites in the C-terminal domain of mouse prion protein: A hybrid (QM/MM) molecular dynamics study. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 1084-1098.	2.6	21
79	Accelerating Rare Reactive Events by Means of a Finite Electronic Temperature. <i>Journal of the American Chemical Society</i> , 2002, 124, 8163-8171.	13.7	20
80	Reductive Hydrogenation of the Aqueous Rutile TiO <sub>2</sub> (110) Surface. <i>Electrochimica Acta</i> , 2015, 179, 658-667.	5.2	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. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 064206.	1.8	19
82	Structure and Mobility of Acetic Acid at the Anatase (101)/Acetonitrile Interface. <i>Journal of Physical Chemistry C</i> , 2014, 118, 6251-6260.	3.1	19
83	A generalized Poisson solver for first-principles device simulations. <i>Journal of Chemical Physics</i> , 2016, 144, 044113.	3.0	18
84	Efficient algorithms for large-scale quantum transport calculations. <i>Journal of Chemical Physics</i> , 2017, 147, 074116.	3.0	18
85	Role of Water, CO <sub>2</sub> , and Noninnocent Ligands in the CO <sub>2</sub> Hydrogenation to Formate by an Ir(III) PNP Pincer Catalyst Evaluated by Static-DFT and ab Initio Molecular Dynamics under Reaction Conditions. <i>Organometallics</i> , 2017, 36, 4908-4919.	2.3	18
86	Correction to "Bulk Liquid Water at Ambient Temperature and Pressure from MP2 Theory". <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3066-3067.	4.6	16
87	Pushing back the limit of <i>ab-initio</i> quantum transport simulations on hybrid supercomputers. , 2015, , .		16
88	First-Principles Monte Carlo Simulations of Reaction Equilibria in Compressed Vapors. <i>ACS Central Science</i> , 2016, 2, 409-415.	11.3	16
89	Ab initiomolecular dynamics study of ascorbic acid in aqueous solution. <i>Molecular Physics</i> , 2007, 105, 17-23.	1.7	14
90	Excess Electrons and Interstitial Li Atoms in TiO <sub>2</sub> Anatase: Properties of the (101) Interface. <i>Journal of Physical Chemistry C</i> , 2015, 119, 15009-15018.	3.1	14

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91	Three- and Four-Center Trans Effects in Triply Bonded Ditungsten Complexes: An ab Initio Molecular Dynamics Study of Compounds with Stoichiometry $W_2Cl_4(NHEt)_2(PMe_3)_2$ . <i>Inorganic Chemistry</i> , 2000, 39, 5553-5560.	4.0	12
92	Speed Limits for Acid-Base Chemistry in Aqueous Solutions. <i>Chimia</i> , 2012, 66, 182-186.	0.6	12
93	Solvation of p-Coumaric Acid in Water. <i>Journal of Physical Chemistry B</i> , 2007, 111, 13591-13599.	2.6	10
94	Nuclear Quantum Effects on Aqueous Electron Attachment and Redox Properties. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1424-1428.	4.6	10
95	A comparison of accelerators for direct energy minimization in electronic structure calculations. <i>Journal of Chemical Physics</i> , 2011, 134, 244104.	3.0	9
96	GridTools: A framework for portable weather and climate applications. <i>SoftwareX</i> , 2021, 15, 100707.	2.6	9
97	Cis-Trans Isomerization in Triply-Bonded Ditungsten Complexes: A Multitude of Possible Pathways. <i>Inorganic Chemistry</i> , 2001, 40, 5780-5786.	4.0	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 $Ba(NO_3)_2$ by Ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry C</i> , 2010, 114, 15042-15048.	3.1	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. <i>CCF Transactions on High Performance Computing</i> , 2021, 3, 407-426.	1.7	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. <i>Chimia</i> , 2007, 61, 155-158.	0.6	6
104	Efficient preconditioning of the electronic structure problem in large scale <i>ab initio</i> molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2015, 142, 244117.	3.0	6
105	Microcanonical RT-TDDFT simulations of realistically extended devices. <i>Journal of Chemical Physics</i> , 2018, 149, 124701.	3.0	4
106	Dynamics of the Bulk Hydrated Electron from Many-Body Wave-Function Theory. <i>Angewandte Chemie</i> , 2019, 131, 3930-3933.	2.0	4
107	Estimating equilibrium properties from non-Hamiltonian dynamics. <i>Journal of Chemical Physics</i> , 2001, 115, 7859-7864.	3.0	2
108	Towards ab-initio simulations of nanowire field-effect transistors. , 2014, , .		2

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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