Michiel Sprik

List of Publications by Year
in descending order

136	11,822	23544	58	26591	107
papers	citations		h-index		g-index

140	140	140	7599
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Free energy from constrained molecular dynamics. Journal of Chemical Physics, 1998, 109, 7737-7744.	1.2	733
2	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
3	A polarizable model for water using distributed charge sites. Journal of Chemical Physics, 1988, 89, 7556-7560.	1.2	471
4	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
5	Molecular model for aqueous ferrousâ€“ferric electron transfer. Journal of Chemical Physics, 1988, 89, 3248-3257.	1.2	417
6	The Silicaâ€“Water Interface: How the Silanols Determine the Surface Acidity and Modulate the Water Properties. Journal of Chemical Theory and Computation, 2012, 8, 1037-1047.	2.3	352
7	Influence of surface topology and electrostatic potential on water/electrode systems. Journal of Chemical Physics, 1995, 102, 511-524.	1.2	332
8	New generalized gradient approximation functionals. Journal of Chemical Physics, 2000, 112, 1670-1678.	1.2	332
9	Liquid Water from First Principles:Â Investigation of Different Sampling Approaches. Journal of Physical Chemistry B, 2004, 108, 12990-12998.	1.2	327
10	Ab Initio Molecular Dynamics Computation of the Infrared Spectrum of Aqueous Uracil. Journal of Physical Chemistry B, 2003, 107, 10344-10358.	1.2	245
11	A densityâ€functional study of the intermolecular interactions of benzene. Journal of Chemical Physics, 1996, 105, 8684-8689.	1.2	238
12	Alignment of electronic energy levels at electrochemical interfaces. Physical Chemistry Chemical Physics, 2012, 14, 11245.	1.3	233
13	Electronic Structure and Solvation of Copper and Silver Ions:Â A Theoretical Picture of a Model Aqueous Redox Reaction. Journal of the American Chemical Society, 2004, 126, 3928-3938.	6.6	196
14	Redox Potentials and Acidity Constants from Density Functional Theory Based Molecular Dynamics. Accounts of Chemical Research, 2014, 47, 3522-3529.	7.6	181
15	Acidity of edge surface sites of montmorillonite and kaolinite. Geochimica Et Cosmochimica Acta, 2013, 117, 180-190.	1.6	180
16	Acidity of the Aqueous Rutile TiO₂(110) Surface from Density Functional Theory Based Molecular Dynamics. Journal of Chemical Theory and Computation, 2010, 6, 880-889.	2.3	179
17	Staging: A sampling technique for the Monte Carlo evaluation of path integrals. Physical Review B, 1985, 31, 4234-4244.	1.1	172
18	Key Steps of the cis-Platin-DNA Interaction:â€‰ Density Functional Theory-Based Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2000, 104, 823-835.	1.2	166

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19	Computation of the pK of liquid water using coordination constraints. Chemical Physics, 2000, 258, 139-150.	0.9	163
20	Ab initio molecular dynamics of ion solvation. The case of Be2+ in water. Chemical Physics Letters, 1997, 273, 360-366.	1.2	159
21	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
22	Redox potentials and pKa for benzoquinone from density functional theory based molecular dynamics. Journal of Chemical Physics, 2009, 131, 154504.	1.2	158
23	Hydrogen bonding and the static dielectric constant in liquid water. Journal of Chemical Physics, 1991, 95, 6762-6769.	1.2	145
24	Vibrational Sum Frequency Generation Spectroscopy of the Water Liquidâ€“Vapor Interface from Density Functional Theory-Based Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2013, 4, 83-87.	2.1	142
25	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
26	Acidity constants from vertical energy gaps: density functional theory based molecular dynamics implementation. Physical Chemistry Chemical Physics, 2008, 10, 5238.	1.3	131
27	Computer simulation of muonium in water. Journal of Chemical Physics, 1984, 80, 5719-5724.	1.2	118
28	Modeling the Oxygen Evolution Reaction on Metal Oxides: The Infuence of Unrestricted DFT Calculations. Journal of Physical Chemistry C, 2014, 118, 4095-4102.	1.5	117
29	Aligning electronic energy levels at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m Physical Review B, 2010, 82, .	1.1	115
30	The oxidation of tyrosine and tryptophan studied by a molecular dynamics normal hydrogen electrode. Journal of Chemical Physics, 2011, 134, 244508.	1.2	115
31	Molecular dynamics simulation of an aqueous sodium octanoate micelle using polarizable surfactant molecules. Langmuir, 1993, 9, 916-926.	1.6	113
32	Diabatic free energy curves and coordination fluctuations for the aqueous Ag+âˆ•Ag2+ redox couple: A biased Born-Oppenheimer molecular dynamics investigation. Journal of Chemical Physics, 2006, 124, 064507.	1.2	112
33	Oxide/water interfaces: how the surface chemistry modifies interfacial water properties. Journal of Physics Condensed Matter, 2012, 24, 124106.	0.7	107
34	Coordination numbers as reaction coordinates in constrained molecular dynamics. Faraday Discussions, 1998, 110, 437-445.	1.6	103
35	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
36	Orientational ordering in solidC70: Predictions from computer simulation. Physical Review Letters, 1992, 69, 1660-1663.	2.9	95

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37	Ab Initio Molecular Dynamics Study of the Reaction of Water with Formaldehyde in Sulfuric Acid Solution. Journal of the American Chemical Society, 1998, 120, 6345-6355.	6.6	90
38	Absolute acidity of clay edge sites from ab-initio simulations. Geochimica Et Cosmochimica Acta, 2012, 94, 1-11.	1.6	89
39	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
40	Second-order elastic constants for the Lennard-Jones solid. Physical Review B, 1984, 29, 4368-4374.	1.1	87
41	Density-functional molecular-dynamics study of the redox reactions of two anionic, aqueous transition-metal complexes. Journal of Chemical Physics, 2005, 122, 234505.	1.2	86
42	Ab Initio Molecular Dynamics Simulation of the Aqueous Ru2+/Ru3+Redox Reaction:Â The Marcus Perspectiveâ€. Journal of Physical Chemistry B, 2005, 109, 6793-6804.	1.2	85
43	Identifying Trapped Electronic Holes at the Aqueous TiO₂ Interface. Journal of Physical Chemistry C, 2014, 118, 5437-5444.	1.5	85
44	Optimization of a distributed Gaussian basis set using simulated annealing: Application to the adiabatic dynamics of the solvated electron. Journal of Chemical Physics, 1988, 89, 1592-1607.	1.2	84
45	Ionic solvation in nonaqueous solvents: the structure of lithium ion and chloride in methanol, ammonia, and methylamine. Journal of the American Chemical Society, 1987, 109, 5900-5904.	6.6	82
46	A Density Functional Study of the Addition of Water to SO3in the Gas Phase and in Aqueous Solution. Journal of Physical Chemistry A, 1998, 102, 2893-2898.	1.1	82
47	Ab InitioMolecular Dynamics for Molecules with Variable Numbers of Electrons. Physical Review Letters, 2002, 88, 213002.	2.9	82
48	Electronic properties of hard and soft ions in solution: Aqueous Na+ and Ag+ compared. Journal of Chemical Physics, 2001, 115, 3454-3468.	1.2	79
49	Absolute pK_a Values and Solvation Structure of Amino Acids from Density Functional Based Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2011, 7, 1951-1961.	2.3	79
50	Aqueous Redox Chemistry and the Electronic Band Structure of Liquid Water. Journal of Physical Chemistry Letters, 2012, 3, 3411-3415.	2.1	76
51	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
52	Effects of third-order susceptibility in sum frequency generation spectra: a molecular dynamics study in liquid water. Physical Chemistry Chemical Physics, 2018, 20, 3040-3053.	1.3	74
53	Study of electron solvation in liquid ammonia using quantum path integral Monte Carlo calculations. Journal of Chemical Physics, 1985, 83, 5802-5809.	1.2	72
54	Surface acidity of 2:1-type dioctahedral clay minerals from first principles molecular dynamics simulations. Geochimica Et Cosmochimica Acta, 2014, 140, 410-417.	1.6	72

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55	Ab Initio Molecular Dynamics Study of Uracil in Aqueous Solution. Journal of Physical Chemistry B, 2004, 108, 7458-7467.	1.2	67
56	Hole Localization and Thermochemistry of Oxidative Dehydrogenation of Aqueous Rutile TiO₂(110). ChemCatChem, 2012, 4, 636-640.	1.8	65
57	Simulation of an excess electron in a hard sphere fluid. Journal of Chemical Physics, 1985, 83, 3042-3049.	1.2	63
58	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
59	Understanding surface acidity of gibbsite with first principles molecular dynamics simulations. Geochimica Et Cosmochimica Acta, 2013, 120, 487-495.	1.6	61
60	Thermal versus electronic broadening in the density of states of liquid water. Chemical Physics Letters, 2003, 376, 68-74.	1.2	59
61	Electron-Ion Interactions and Ionization in a Polar Solvent. Physical Review Letters, 1986, 56, 2326-2329.	2.9	58
62	The torsional potential of perfluoronâ€alkanes: A density functional study. Journal of Chemical Physics, 1996, 104, 3692-3700.	1.2	56
63	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
64	Acidity constants from DFT-based molecular dynamics simulations. Journal of Physics Condensed Matter, 2010, 22, 284116.	0.7	54
65	Coupling of Surface Chemistry and Electric Double Layer at TiO₂ Electrochemical Interfaces. Journal of Physical Chemistry Letters, 2019, 10, 3871-3876.	2.1	53
66	A Classical Point Charge Model Study of System Size Dependence of Oxidation and Reorganization Free Energies in Aqueous Solution. Journal of Physical Chemistry B, 2008, 112, 257-269.	1.2	49
67	Computing the dielectric constant of liquid water at constant dielectric displacement. Physical Review B, 2016, 93, .	1.1	49
68	Simulating Electrochemical Systems by Combining the Finite Field Method with a Constant Potential Electrode. Physical Review Letters, 2019, 123, 195501.	2.9	48
69	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
70	Free Energy of Oxidation of Metal Aqua Ions by an Enforced Change of Coordination. Journal of Physical Chemistry B, 2004, 108, 6529-6535.	1.2	45
71	Computer simulation of a quantum particle in a quenched disordered system: Direct observation of Lifshitz traps. Physical Review B, 1985, 32, 545-547.	1.1	44
72	Density functional calculation of the electronic absorption spectrum of Cu+ and Ag+ aqua ions. Journal of Chemical Physics, 2004, 121, 11885-11899.	1.2	43

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73	Long-Range Solvent Effects on the Orbital Interaction Mechanism of Water Acidity Enhancement in Metal Ion Solutions:Â A Comparative Study of the Electronic Structure of Aqueous Mg and Zn Dications. Journal of Physical Chemistry B, 2006, 110, 11444-11453.	1.2	43
74	Finite field methods for the supercell modeling of charged insulator/electrolyte interfaces. Physical Review B, 2016, 94, .	1.1	42
75	Theoretical pKaestimates for solvated P(OH)5from coordination constrained Carâ€“Parrinello molecular dynamics. Physical Chemistry Chemical Physics, 2003, 5, 2612-2618.	1.3	41
76	Structure of Solid Poly(tetrafluoroethylene):â€‰ A Computer Simulation Study of Chain Orientational, Translational, and Conformational Disorder. Journal of Physical Chemistry B, 1997, 101, 2745-2749.	1.2	40
77	Adiabatic dynamics of the solvated electron in liquid ammonia. Journal of Chemical Physics, 1989, 91, 5665-5671.	1.2	39
78	Solution Structures and Acidity Constants of Molybdic Acid. Journal of Physical Chemistry Letters, 2013, 4, 2926-2930.	2.1	39
79	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
80	Free energies of absorption of alkali ions onto beidellite and montmorillonite surfaces from constrained molecular dynamics simulations. Geochimica Et Cosmochimica Acta, 2012, 91, 109-119.	1.6	38
81	Modelling electrochemical systems with finite field molecular dynamics. JPhys Energy, 2020, 2, 032005.	2.3	38
82	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
83	Ab initio molecular dynamics simulation of redox reactions in solution. Computer Physics Communications, 2005, 169, 256-261.	3.0	35
84	The ionization potential of aqueous hydroxide computed using many-body perturbation theory. Journal of Chemical Physics, 2014, 141, 034501.	1.2	35
85	Interfacial structures and acidity of edge surfaces of ferruginous smectites. Geochimica Et Cosmochimica Acta, 2015, 168, 293-301.	1.6	34
86	Constrained reaction coordinate dynamics for systems with constraints. Molecular Physics, 2003, 101, 2885-2894.	0.8	31
87	On the Position of the Highest Occupied Molecular Orbital in Aqueous Solutions of Simple Ions. ChemPhysChem, 2005, 6, 1805-1808.	1.0	31
88	Electron attachment to ammonia clusters: A study using path integral Monte Carlo calculations. Journal of Chemical Physics, 1988, 89, 4918-4923.	1.2	30
89	Electronic excitation spectra from time-dependent density functional response theory using plane-wave methods. Chemical Physics Letters, 2000, 330, 563-569.	1.2	30
90	Toward a Monte Carlo program for simulating vaporâ€“liquid phase equilibria from first principles. Computer Physics Communications, 2005, 169, 289-294.	3.0	29

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91	From Solvent Fluctuations to Quantitative Redox Properties of Quinones in Methanol and Acetonitrile. Angewandte Chemie - International Edition, 2006, 45, 1936-1938.	7.2	29
92	Ligand Field Effects on the Aqueous Ru(III)/Ru(II) Redox Couple from an All-Atom Density Functional Theory Perspective. Journal of Chemical Theory and Computation, 2006, 2, 1403-1415.	2.3	28
93	Simulation of the cubic to orthorhombic phase transition in potassium cyanide. Journal of Chemical Physics, 1985, 83, 3638-3644.	1.2	27
94	Free energy calculation of water addition coupled to reduction of aqueous RuO4â˜. Journal of Chemical Physics, 2007, 126, 204506.	1.2	27
95	Solvation of electrons, atoms and ions in liquid ammonia. Faraday Discussions of the Chemical Society, 1988, 85, 373.	2.2	26
96	Aqueous Transition-Metal Cations as Impurities in a Wide Gap Oxide: The Cu²⁺/Cu⁺ and Ag²⁺/Ag⁺ Redox Couples Revisited. Journal of Physical Chemistry B, 2015, 119, 1152-1163.	1.2	24
97	Ab initiomolecular dynamics simulation of liquids and solutions. Journal of Physics Condensed Matter, 1996, 8, 9405-9409.	0.7	23
98	Pressure Effects on Hydrogen Bonding in the Disordered Phase of Solid HBr. Physical Review Letters, 1998, 81, 4416-4419.	2.9	22
99	Temperature dependence of interfacial structures and acidity of clay edge surfaces. Geochimica Et Cosmochimica Acta, 2015, 160, 91-99.	1.6	22
100	Pressure-induced structural and chemical changes of solid HBr. Journal of Chemical Physics, 1999, 111, 1595-1607.	1.2	21
101	Living polymers Ab initio molecular dynamics study of the initiation step in the polymerization of isoprene induced by ethyl lithium. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 501-508.	1.7	20
102	Reductive Hydrogenation of the Aqueous Rutile TiO 2 (110) Surface. Electrochimica Acta, 2015, 179, 658-667.	2.6	20
103	Density Functional Theory Calculation of the Band Alignment of (101Ì…0) In_xGa_{1â€“x}N/Water Interfaces. Journal of Physical Chemistry B, 2016, 120, 1928-1939.	1.2	20
104	Hydration, acidity and metal complexing of polysulfide species: A first principles molecular dynamics study. Chemical Physics Letters, 2013, 563, 9-14.	1.2	19
105	Finite electric displacement simulations of polar ionic solid-electrolyte interfaces: Application to NaCl(111)/aqueous NaCl solution. Journal of Chemical Physics, 2019, 150, 041716.	1.2	19
106	Application of path integral simulations to the study of electron solvation in polar fluids. Computer Physics Reports, 1988, 7, 147-166.	2.3	17
107	Computing Surface Acidity Constants of Proton Hopping Groups from Density Functional Theory-Based Molecular Dynamics: Application to the SnO₂(110)/H₂O Interface. Journal of Chemical Theory and Computation, 2020, 16, 6520-6527.	2.3	16
108	Molecular Simulation Study of Hydrated Na-Rectorite. Langmuir, 2015, 31, 2008-2013.	1.6	15

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109	Electronic Energy Levels and Band Alignment for Aqueous Phenol and Phenolate from First Principles. Journal of Physical Chemistry B, 2015, 119, 9651-9660.	1.2	15
110	Charge compensation at the interface between the polar NaCl(111) surface and a NaCl aqueous solution. Journal of Chemical Physics, 2017, 147, 104702.	1.2	15
111	Finite field formalism for bulk electrolyte solutions. Journal of Chemical Physics, 2019, 151, .	1.2	15
112	Computational Amperometry of Nanoscale Capacitors in Molecular Simulations. Journal of Physical Chemistry Letters, 2021, 12, 4357-4361.	2.1	15
113	Finite Maxwell field and electric displacement Hamiltonians derived from a current dependent Lagrangian. Molecular Physics, 2018, 116, 3114-3120.	0.8	14
114	Thermodynamic Investigation of Proton/Electron Interplay on the Pourbaix Diagram at the TiO₂/Electrolyte Interface. Journal of Physical Chemistry C, 2020, 124, 19003-19014.	1.5	14
115	Electromechanics of the liquid water vapour interface. Physical Chemistry Chemical Physics, 2020, 22, 10676-10686.	1.3	14
116	Orientational ordering in solid parahydrogen and orthodeuterium. Journal of Chemical Physics, 1984, 81, 6207-6213.	1.2	13
117	First Principles Study of Alkaliâ^'Tyrosine Complexes: Alkali Solvation and Redox Properties. Journal of Chemical Theory and Computation, 2008, 4, 1049-1056.	2.3	13
118	Ab initiomolecular dynamics simulation of liquids and solutions. Journal of Physics Condensed Matter, 2000, 12, A161-A163.	0.7	12
119	Molecular dynamics study of electron gas models for liquid water. Molecular Physics, 2003, 101, 1183-1198.	0.8	12
120	Activation energy for a model ferrous-ferric half reaction from transition path sampling. Journal of Chemical Physics, 2012, 136, 034506.	1.2	11
121	Editorial: A Tribute to Michele Parrinello: From Physics via Chemistry to Biology. ChemPhysChem, 2005, 6, 1671-1676.	1.0	9
122	A correlated variational wave function for the orientational ground state of solid methane. Journal of Chemical Physics, 1984, 80, 1988-1999.	1.2	8
123	Folding of model heteropolymers by configurational-bias Monte Carlo. Chemical Physics Letters, 1992, 199, 220-224.	1.2	8
124	Competing interactions in self-assembled monolayers containing peptide groups: molecular dynamics studies of long-chain perfluoro mercaptans on Au(111). Journal of Materials Chemistry, 1994, 4, 793-803.	6.7	8
125	Hydrogen Elimination and Solid-State Reaction in Hydrogen-Bonded Systems under Pressure:â€‰ The Case of HBr. Journal of Physical Chemistry B, 2000, 104, 11801-11804.	1.2	7
126	Time-Dependent Density Functional Theory Description of On-Site Electron Repulsion and Ligand Field Effects in the Optical Spectrum of Hexaaquoruthenium(II) in Solution. Journal of Physical Chemistry B, 2005, 109, 12222-12226.	1.2	7

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127	Electron Transfer Properties from Atomistic Simulations and Density Functional Theory. Chimia, 2007, 61, 155-158.	0.3	6
128	Pressure-induced structural changes of HBr. Physica B: Condensed Matter, 1999, 265, 101-104.	1.3	5
129	Electric-field-based Poisson-Boltzmann theory: Treating mobile charge as polarization. Physical Review E, 2021, 103, 022803.	0.8	4
130	Soluteâ€“Solvent Charge-Transfer Excitations and Optical Absorption of Hydrated Hydroxide from Time-Dependent Density-Functional Theory. Journal of Chemical Theory and Computation, 2014, 10, 2465-2470.	2.3	3
131	The temperature dependence of the symmetry factor for a model Fe³⁺(aq)/Fe²⁺(aq) redox half reaction. Molecular Physics, 2015, 113, 2463-2475.	0.8	3
132	Band positions of anatase (001) and (101) surfaces in contact with water from density functional theory. Journal of Chemical Physics, 2020, 152, 194706.	1.2	3
133	Chemomechanical equilibrium at the interface between a simple elastic solid and its liquid phase. Journal of Chemical Physics, 2021, 155, 244701.	1.2	3
134	Ordering of fractional monolayers of H2O on Ni(110). Surface Science Letters, 1992, 279, L185-L190.	0.1	0
135	Density functional techniques for simulation of chemical reactions. , 1998, , .		0
136	Readive liquids from first principles. Europhysics News, 2000, 31, 9-10.	0.1	0