Michiel Sprik

List of Publications by Citations

134 papers	10,480 citations	56 h-index	101 g-index
140 ext. papers	11,156 ext. citations	4.7 avg, IF	6.44 L-index

#	Paper	IF	Citations
134	Free energy from constrained molecular dynamics. *Journal of Chemical Physics*, **1998**, 109, 7737-7744	3.9	633
133	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
132	A polarizable model for water using distributed charge sites. *Journal of Chemical Physics*, **1988**, 89, 7556-7560	3.9	445
131	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
130	Molecular model for aqueous ferrous–ferric electron transfer. *Journal of Chemical Physics*, **1988**, 89, 3248-3257	3.9	386
129	New generalized gradient approximation functionals. *Journal of Chemical Physics*, **2000**, 112, 1670-1678	3.9	312
128	Liquid Water from First Principles: Investigation of Different Sampling Approaches. *Journal of Physical Chemistry B*, **2004**, 108, 12990-12998	3.4	309
127	The Silica-Water Interface: How the Silanols Determine the Surface Acidity and Modulate the Water Properties. *Journal of Chemical Theory and Computation*, **2012**, 8, 1037-47	6.4	279
126	Influence of surface topology and electrostatic potential on water/electrode systems. *Journal of Chemical Physics*, **1995**, 102, 511-524	3.9	268
125	Ab Initio Molecular Dynamics Computation of the Infrared Spectrum of Aqueous Uracil. *Journal of Physical Chemistry B*, **2003**, 107, 10344-10358	3.4	227
124	A density-functional study of the intermolecular interactions of benzene. *Journal of Chemical Physics*, **1996**, 105, 8684-8689	3.9	224
123	Alignment of electronic energy levels at electrochemical interfaces. *Physical Chemistry Chemical Physics*, **2012**, 14, 11245-67	3.6	185
122	Electronic structure and solvation of copper and silver ions: a theoretical picture of a model aqueous redox reaction. *Journal of the American Chemical Society*, **2004**, 126, 3928-38	16.4	183
121	Staging: A sampling technique for the Monte Carlo evaluation of path integrals. *Physical Review B*, **1985**, 31, 4234-4244	3.3	168
120	Acidity of the Aqueous Rutile TiO2(110) Surface from Density Functional Theory Based Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2010**, 6, 880-9	6.4	159
119	Key Steps of the cis-Platin-DNA Interaction: Density Functional Theory-Based Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2000**, 104, 823-835	3.4	158
118	Acidity of edge surface sites of montmorillonite and kaolinite. *Geochimica Et Cosmochimica Acta*, **2013**, 117, 180-190	5.5	146

117	A molecular dynamics study of the hydroxyl radical in solution applying self-interaction-corrected density functional methods. *Physical Chemistry Chemical Physics*, **2005**, 7, 1363-7	3.6	146
116	Ab initio molecular dynamics of ion solvation. The case of Be2+ in water. *Chemical Physics Letters*, **1997**, 273, 360-366	2.5	144
115	Computation of the pK of liquid water using coordination constraints. *Chemical Physics*, **2000**, 258, 139-150	2.9	141
114	Redox potentials and pKa for benzoquinone from density functional theory based molecular dynamics. *Journal of Chemical Physics*, **2009**, 131, 154504	3.9	138
113	Hydrogen bonding and the static dielectric constant in liquid water. *Journal of Chemical Physics*, **1991**, 95, 6762-6769	3.9	135
112	Redox potentials and acidity constants from density functional theory based molecular dynamics. *Accounts of Chemical Research*, **2014**, 47, 3522-9	24.3	134
111	Vibrational Sum Frequency Generation Spectroscopy of the Water Liquid-Vapor Interface from Density Functional Theory-Based Molecular Dynamics Simulations. *Journal of Physical Chemistry Letters*, **2013**, 4, 83-7	6.4	128
110	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
109	Acidity constants from vertical energy gaps: density functional theory based molecular dynamics implementation. *Physical Chemistry Chemical Physics*, **2008**, 10, 5238-49	3.6	113
108	Computer simulation of muonium in water. *Journal of Chemical Physics*, **1984**, 80, 5719-5724	3.9	111
107	Aligning electronic energy levels at the TiO2/H2O interface. *Physical Review B*, **2010**, 82,	3.3	108
106	Molecular dynamics simulation of an aqueous sodium octanoate micelle using polarizable surfactant molecules. *Langmuir*, **1993**, 9, 916-926	4	105
105	Diabatic free energy curves and coordination fluctuations for the aqueous Ag+Ag2+ redox couple: a biased Born-Oppenheimer molecular dynamics investigation. *Journal of Chemical Physics*, **2006**, 124, 64507	3.9	100
104	The oxidation of tyrosine and tryptophan studied by a molecular dynamics normal hydrogen electrode. *Journal of Chemical Physics*, **2011**, 134, 244508	3.9	98
103	Coordination numbers as reaction coordinates in constrained molecular dynamics. *Faraday Discussions*, **1998**, 110, 437-445	3.6	94
102	Oxide/water interfaces: how the surface chemistry modifies interfacial water properties. *Journal of Physics Condensed Matter*, **2012**, 24, 124106	1.8	90
101	Orientational ordering in solid C70: Predictions from computer simulation. *Physical Review Letters*, **1992**, 69, 1660-1663	7.4	90
100	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

99	Modeling the Oxygen Evolution Reaction on Metal Oxides: The Influence of Unrestricted DFT Calculations. *Journal of Physical Chemistry C*, **2014**, 118, 4095-4102	3.8	81
98	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	16.4	81
97	Calculation of redox properties: understanding short- and long-range effects in rubredoxin. *Journal of Physical Chemistry B*, **2007**, 111, 3969-76	3.4	81
96	Density-functional molecular-dynamics study of the redox reactions of two anionic, aqueous transition-metal complexes. *Journal of Chemical Physics*, **2005**, 122, 234505	3.9	81
95	Ab initio molecular dynamics simulation of the aqueous Ru2+/Ru3+ redox reaction: the Marcus perspective. *Journal of Physical Chemistry B*, **2005**, 109, 6793-804	3.4	79
94	Electronic properties of hard and soft ions in solution: Aqueous Na+ and Ag+ compared. *Journal of Chemical Physics*, **2001**, 115, 3454-3468	3.9	78
93	Ab initio molecular dynamics for molecules with variable numbers of electrons. *Physical Review Letters*, **2002**, 88, 213002	7.4	77
92	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	16.4	76
91	Second-order elastic constants for the Lennard-Jones solid. *Physical Review B*, **1984**, 29, 4368-4374	3.3	76
90	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	3.9	75
89	Absolute acidity of clay edge sites from ab-initio simulations. *Geochimica Et Cosmochimica Acta*, **2012**, 94, 1-11	5.5	74
88	Identifying Trapped Electronic Holes at the Aqueous TiO2 Interface. *Journal of Physical Chemistry C*, **2014**, 118, 5437-5444	3.8	72
87	Absolute pKa Values and Solvation Structure of Amino Acids from Density Functional Based Molecular Dynamics Simulation. *Journal of Chemical Theory and Computation*, **2011**, 7, 1951-61	6.4	70
86	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	2.8	70
85	Aqueous Redox Chemistry and the Electronic Band Structure of Liquid Water. *Journal of Physical Chemistry Letters*, **2012**, 3, 3411-5	6.4	67
84	Ab Initio Molecular Dynamics Study of Uracil in Aqueous Solution. *Journal of Physical Chemistry B*, **2004**, 108, 7458-7467	3.4	67
83	Study of electron solvation in liquid ammonia using quantum path integral Monte Carlo calculations. *Journal of Chemical Physics*, **1985**, 83, 5802-5809	3.9	67
82	Aligning electronic and protonic energy levels of proton-coupled electron transfer in water oxidation on aqueous TiO*Angewandte Chemie - International Edition*, **2014**, 53, 12046-50	16.4	64

81	Surface acidity of 2:1-type dioctahedral clay minerals from first principles molecular dynamics simulations. *Geochimica Et Cosmochimica Acta*, **2014**, 140, 410-417	5.5	63
80	Simulation of an excess electron in a hard sphere fluid. *Journal of Chemical Physics*, **1985**, 83, 3042-3049	3.9	61
79	Hole Localization and Thermochemistry of Oxidative Dehydrogenation of Aqueous Rutile TiO2(110). *ChemCatChem*, **2012**, 4, 636-640	5.2	56
78	Thermal versus electronic broadening in the density of states of liquid water. *Chemical Physics Letters*, **2003**, 376, 68-74	2.5	56
77	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	3.6	53
76	Electron-ion interactions and ionization in a polar solvent. *Physical Review Letters*, **1986**, 56, 2326-2329	7.4	53
75	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
74	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
73	The torsional potential of perfluoro n-alkanes: A density functional study. *Journal of Chemical Physics*, **1996**, 104, 3692-3700	3.9	48
72	Acidity constants from DFT-based molecular dynamics simulations. *Journal of Physics Condensed Matter*, **2010**, 22, 284116	1.8	47
71	Understanding surface acidity of gibbsite with first principles molecular dynamics simulations. *Geochimica Et Cosmochimica Acta*, **2013**, 120, 487-495	5.5	46
70	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, 6046-7	16.4	45
69	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, 257-69	3.4	45
68	Computer simulation of a quantum particle in a quenched disordered system: Direct observation of Lifshitz traps. *Physical Review B*, **1985**, 32, 545-547	3.3	42
67	Long-range solvent effects on the orbital interaction mechanism of water acidity enhancement in metal ion solutions: a comparative study of the electronic structure of aqueous Mg and Zn dications. *Journal of Physical Chemistry B*, **2006**, 110, 11444-53	3.4	41
66	Free Energy of Oxidation of Metal Aqua Ions by an Enforced Change of Coordination *Journal of Physical Chemistry B*, **2004**, 108, 6529-6535	3.4	41
65	Density functional calculation of the electronic absorption spectrum of Cu+ and Ag+ aqua ions. *Journal of Chemical Physics*, **2004**, 121, 11885-99	3.9	40
64	Theoretical pKa estimates for solvated P(OH)5 from coordination constrained Car–Parrinello molecular dynamics. *Physical Chemistry Chemical Physics*, **2003**, 5, 2612-2618	3.6	38

63	Structure of Solid Poly(tetrafluoroethylene): A Computer Simulation Study of Chain Orientational, Translational, and Conformational Disorder. *Journal of Physical Chemistry B*, **1997**, 101, 2745-2749	3.4	37
62	Density functional theory study of tetrathiafulvalene and thianthrene in acetonitrile: structure, dynamics, and redox properties. *Journal of Physical Chemistry B*, **2006**, 110, 3614-23	3.4	37
61	Adiabatic dynamics of the solvated electron in liquid ammonia. *Journal of Chemical Physics*, **1989**, 91, 5665-5671	3.9	37
60	Coupling of Surface Chemistry and Electric Double Layer at TiO Electrochemical Interfaces. *Journal of Physical Chemistry Letters*, **2019**, 10, 3871-3876	6.4	36
59	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	4.1	35
58	Computing the dielectric constant of liquid water at constant dielectric displacement. *Physical Review B*, **2016**, 93,	3.3	33
57	Solution Structures and Acidity Constants of Molybdic Acid. *Journal of Physical Chemistry Letters*, **2013**, 4, 2926-2930	6.4	33
56	Ab initio molecular dynamics simulation of redox reactions in solution. *Computer Physics Communications*, **2005**, 169, 256-261	4.2	33
55	The ionization potential of aqueous hydroxide computed using many-body perturbation theory. *Journal of Chemical Physics*, **2014**, 141, 034501	3.9	32
54	Modelling electrochemical systems with finite field molecular dynamics. *JPhys Energy*, **2020**, 2, 032005	4.9	32
53	Simulating Electrochemical Systems by Combining the Finite Field Method with a Constant Potential Electrode. *Physical Review Letters*, **2019**, 123, 195501	7.4	30
52	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	5.5	30
51	On the position of the highest occupied molecular orbital in aqueous solutions of simple ions. *ChemPhysChem*, **2005**, 6, 1805-8	3.2	30
50	Finite field methods for the supercell modeling of charged insulator/electrolyte interfaces. *Physical Review B*, **2016**, 94,	3.3	30
49	Constrained reaction coordinate dynamics for systems with constraints. *Molecular Physics*, **2003**, 101, 2885-2894	1.7	29
48	Electron attachment to ammonia clusters: A study using path integral Monte Carlo calculations. *Journal of Chemical Physics*, **1988**, 89, 4918-4923	3.9	28
47	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, 1403-15	6.4	26
46	Interfacial structures and acidity of edge surfaces of ferruginous smectites. *Geochimica Et Cosmochimica Acta*, **2015**, 168, 293-301	5.5	25

45	From solvent fluctuations to quantitative redox properties of quinones in methanol and acetonitrile. *Angewandte Chemie - International Edition*, **2006**, 45, 1936-8	16.4	25
44	Free energy calculation of water addition coupled to reduction of aqueous RuO4-. *Journal of Chemical Physics*, **2007**, 126, 204506	3.9	25
43	Toward a Monte Carlo program for simulating vapor□liquid phase equilibria from first principles. *Computer Physics Communications*, **2005**, 169, 289-294	4.2	25
42	Electronic excitation spectra from time-dependent density functional response theory using plane-wave methods. *Chemical Physics Letters*, **2000**, 330, 563-569	2.5	23
41	Ab initiomolecular dynamics simulation of liquids and solutions. *Journal of Physics Condensed Matter*, **1996**, 8, 9405-9409	1.8	23
40	Solvation of electrons, atoms and ions in liquid ammonia. *Faraday Discussions of the Chemical Society*, **1988**, 85, 373		23
39	Aqueous transition-metal cations as impurities in a wide gap oxide: the Cu(2+)/Cu(+) and Ag(2+)/Ag(+) redox couples revisited. *Journal of Physical Chemistry B*, **2015**, 119, 1152-63	3.4	22
38	Simulation of the cubic to orthorhombic phase transition in potassium cyanide. *Journal of Chemical Physics*, **1985**, 83, 3638-3644	3.9	21
37	Temperature dependence of interfacial structures and acidity of clay edge surfaces. *Geochimica Et Cosmochimica Acta*, **2015**, 160, 91-99	5.5	20
36	Living polymers. *Journal of the Chemical Society, Faraday Transactions*, **1998**, 94, 501-508		20
35	Reductive Hydrogenation of the Aqueous Rutile TiO2(110) Surface. *Electrochimica Acta*, **2015**, 179, 658-667		18
34	Pressure Effects on Hydrogen Bonding in the Disordered Phase of Solid HBr. *Physical Review Letters*, **1998**, 81, 4416-4419	7.4	18
33	Pressure-induced structural and chemical changes of solid HBr. *Journal of Chemical Physics*, **1999**, 111, 1595-1607	3.9	18
32	Application of path integral simulations to the study of electron solvation in polar fluids. *Computer Physics Reports*, **1988**, 7, 147-166		16
31	Electronic Energy Levels and Band Alignment for Aqueous Phenol and Phenolate from First Principles. *Journal of Physical Chemistry B*, **2015**, 119, 9651-60	3.4	15
30	Charge compensation at the interface between the polar NaCl(111) surface and a NaCl aqueous solution. *Journal of Chemical Physics*, **2017**, 147, 104702	3.9	15
29	Finite electric displacement simulations of polar ionic solid-electrolyte interfaces: Application to NaCl(111)/aqueous NaCl solution. *Journal of Chemical Physics*, **2019**, 150, 041716	3.9	14
28	Aligning Electronic and Protonic Energy Levels of Proton-Coupled Electron Transfer in Water Oxidation on Aqueous TiO2. *Angewandte Chemie*, **2014**, 126, 12242-12246	3.6	13

27	Hydration, acidity and metal complexing of polysulfide species: A first principles molecular dynamics study. *Chemical Physics Letters*, **2013**, 563, 9-14	2.5	12
26	Molecular simulation study of hydrated Na-rectorite. *Langmuir*, **2015**, 31, 2008-13	4	12
25	First Principles Study of Alkali-Tyrosine Complexes: Alkali Solvation and Redox Properties. *Journal of Chemical Theory and Computation*, **2008**, 4, 1049-56	6.4	12
24	Electromechanics of the liquid water vapour interface. *Physical Chemistry Chemical Physics*, **2020**, 22, 10676-10686	3.6	11
23	Density Functional Theory Calculation of the Band Alignment of (101 0) In(x)Ga(1-x)N/Water Interfaces. *Journal of Physical Chemistry B*, **2016**, 120, 1928-39	3.4	11
22	Molecular dynamics study of electron gas models for liquid water. *Molecular Physics*, **2003**, 101, 1183-1198	1.7	11
21	Ab initiomolecular dynamics simulation of liquids and solutions. *Journal of Physics Condensed Matter*, **2000**, 12, A161-A163	1.8	11
20	Orientational ordering in solid parahydrogen and orthodeuterium. *Journal of Chemical Physics*, **1984**, 81, 6207-6213	3.9	11
19	Finite field formalism for bulk electrolyte solutions. *Journal of Chemical Physics*, **2019**, 151, 064506	3.9	10
18	Activation energy for a model ferrous-ferric half reaction from transition path sampling. *Journal of Chemical Physics*, **2012**, 136, 034506	3.9	10
17	Finite Maxwell field and electric displacement Hamiltonians derived from a current dependent Lagrangian. *Molecular Physics*, **2018**, 116, 3114-3120	1.7	9
16	Computing Surface Acidity Constants of Proton Hopping Groups from Density Functional Theory-Based Molecular Dynamics: Application to the SnO(110)/HO Interface. *Journal of Chemical Theory and Computation*, **2020**, 16, 6520-6527	6.4	8
15	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		7
14	Folding of model heteropolymers by configurational-bias Monte Carlo. *Chemical Physics Letters*, **1992**, 199, 220-224	2.5	7
13	A correlated variational wave function for the orientational ground state of solid methane. *Journal of Chemical Physics*, **1984**, 80, 1988-1999	3.9	7
12	Thermodynamic Investigation of Proton/Electron Interplay on the Pourbaix Diagram at the TiO2/Electrolyte Interface. *Journal of Physical Chemistry C*, **2020**, 124, 19003-19014	3.8	7
11	Electron Transfer Properties from Atomistic Simulations and Density Functional Theory. *Chimia*, **2007**, 61, 155-158	1.3	6
10	Hydrogen Elimination and Solid-State Reaction in Hydrogen-Bonded Systems under Pressure: The Case of HBr. *Journal of Physical Chemistry B*, **2000**, 104, 11801-11804	3.4	6

List of Publications

9	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, 12222-6	3.4	5
8	Computational Amperometry of Nanoscale Capacitors in Molecular Simulations. *Journal of Physical Chemistry Letters*, **2021**, 12, 4357-4361	6.4	5
7	Solute-Solvent Charge-Transfer Excitations and Optical Absorption of Hydrated Hydroxide from Time-Dependent Density-Functional Theory. *Journal of Chemical Theory and Computation*, **2014**, 10, 2465-70	6.4	3
6	Pressure-induced structural changes of HBr. *Physica B: Condensed Matter*, **1999**, 265, 101-104	2.8	3
5	The temperature dependence of the symmetry factor for a model Fe3+(aq)/Fe2+(aq) redox half reaction. *Molecular Physics*, **2015**, 113, 2463-2475	1.7	2
4	Band positions of anatase (001) and (101) surfaces in contact with water from density functional theory. *Journal of Chemical Physics*, **2020**, 152, 194706	3.9	1
3	Electric-field-based Poisson-Boltzmann theory: Treating mobile charge as polarization. *Physical Review E*, **2021**, 103, 022803	2.4	1
2	Chemomechanical equilibrium at the interface between a simple elastic solid and its liquid phase.. *Journal of Chemical Physics*, **2021**, 155, 244701	3.9	0
1	Ordering of fractional monolayers of H2O on Ni(110). *Surface Science Letters*, **1992**, 279, L185-L190		