Markus Meuwly

List of Publications by Year
in descending order

186 papers	5,225 citations	101543 36 h-index	133252 59 g-index
196 all docs	196 docs citations	196 times ranked	3827 citing authors

#	Article	IF	Citations
1	The functional role of the hemoglobin-water interface. Molecular Aspects of Medicine, 2022, 84, 101042.	6.4	2
2	Transfer learned potential energy surfaces: accurate anharmonic vibrational dynamics and dissociation energies for the formic acid monomer and dimer. Physical Chemistry Chemical Physics, 2022, 24, 5269-5281.	2.8	15
3	Machine learning product state distributions from initial reactant states for a reactive atomâ€“diatom collision system. Journal of Chemical Physics, 2022, 156, 034301.	3.0	10
4	Cross-Correlated Motions in Azidolysozyme. Molecules, 2022, 27, 839.	3.8	2
5	Solvent Effects on the Menshutkin Reaction. Journal of Physical Chemistry B, 2022, 126, 1951-1961.	2.6	8
6	Site-selective dynamics of ligand-free and ligand-bound azidolysozyme. Journal of Chemical Physics, 2022, 156, 105105.	3.0	3
7	Photodissociation dynamics of N3+. Journal of Chemical Physics, 2022, 156, 124307.	3.0	0
8	Atomistic Simulations for Reactions and Vibrational Spectroscopy in the Era of Machine Learningâ”€Quo Vadis?. Journal of Physical Chemistry B, 2022, 126, 2155-2167.	2.6	8
9	Mechanistic Insight into the Precursor Chemistry of ZrO₂and HfO₂Nanocrystals; towards Size-Tunable Syntheses. Jacs Au, 2022, 2, 827-838.	7.9	6
10	Quantitative molecular simulations. Physical Chemistry Chemical Physics, 2022, 24, 12767-12786.	2.8	3
11	Double proton transfer in hydrated formic acid dimer: Interplay of spatial symmetry and solvent-generated force on reactivity. Physical Chemistry Chemical Physics, 2022, 24, 13869-13882.	2.8	7
12	Reactive atomistic simulations of Diels-Alder-type reactions: conformational and dynamic effects in the polar cycloaddition of 2,3-dibromobutadiene radical ions with maleic anhydride. Molecular Physics, 2021, 119, e1825852.	1.7	3
13	Spectroscopy, Dynamics, and Hydration of S-Nitrosylated Myoglobin. Journal of Physical Chemistry B, 2021, 125, 4262-4273.	2.6	6
14	Site-selective dynamics of azidolysozyme. Journal of Chemical Physics, 2021, 154, 165101.	3.0	8
15	Transfer Learning to CCSD(T): Accurate Anharmonic Frequencies from Machine Learning Models. Journal of Chemical Theory and Computation, 2021, 17, 3687-3699.	5.3	20
16	Machine Learning for Chemical Reactions. Chemical Reviews, 2021, 121, 10218-10239.	47.7	166
17	Impact of the Characteristics of Quantum Chemical Databases on Machine Learning Prediction of Tautomerization Energies. Journal of Chemical Theory and Computation, 2021, 17, 4769-4785.	5.3	12
18	Genesis of Polyatomic Molecules in Dark Clouds: CO2 Formation on Cold Amorphous Solid Water. Journal of Physical Chemistry Letters, 2021, 12, 6781-6787.	4.6	7

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19	Multipolar Force Fields for Amide-I Spectroscopy from Conformational Dynamics of the Alanine Trimer. Journal of Physical Chemistry B, 2021, 125, 10928-10938.	2.6	6
20	The C(³P) + O₂(³Î£_g^{â^'}) â†' CO₂ â†" CO(¹Î£⁺) + O(¹D)/O(³P) reaction: thermal and vibrational relaxation rates from 15 K to 20â€‰000 K. Physical Chemistry Chemical Physics, 2021, 23, 11251-11263.	2.8	10
21	Thermal and Vibrationally Activated Decomposition of the syn-CH₃CHOO Criegee Intermediate. ACS Earth and Space Chemistry, 2021, 5, 3396-3406.	2.7	8
22	Energy Redistribution Following CO2 Formation on Cold Amorphous Solid Water. Frontiers in Chemistry, 2021, 9, 827085.	3.6	6
23	Machine Learning Models of Vibrating H₂CO: Comparing Reproducing Kernels, FCHL, and PhysNet. Journal of Physical Chemistry A, 2020, 124, 8853-8865.	2.5	24
24	Polarizable Multipolar Molecular Dynamics Using Distributed Point Charges. Journal of Chemical Theory and Computation, 2020, 16, 7267-7280.	5.3	8
25	Machine Learning for Observables: Reactant to Product State Distributions for Atomâ€"Diatom Collisions. Journal of Physical Chemistry A, 2020, 124, 7177-7190.	2.5	12
26	Accurate reproducing kernel-based potential energy surfaces for the triplet ground states of N₂O and dynamics for the N + NO â†" O + N₂ and N₂ + O â†' 2N + O reactions. Physical Chemistry Chemical Physics, 2020, 22, 18488-18498.	2.8	24
27	N3+: Full-dimensional ground state potential energy surface, vibrational energy levels, and dynamics. Journal of Chemical Physics, 2020, 153, 044302.	3.0	7
28	Permutationally Invariant, Reproducing Kernel-Based Potential Energy Surfaces for Polyatomic Molecules: From Formaldehyde to Acetone. Journal of Chemical Theory and Computation, 2020, 16, 5474-5484.	5.3	37
29	Dynamics on Multiple Potential Energy Surfaces: Quantitative Studies of Elementary Processes Relevant to Hypersonics. Journal of Physical Chemistry A, 2020, 124, 6255-6269.	2.5	13
30	Isomerization and decomposition reactions of acetaldehyde relevant to atmospheric processes from dynamics simulations on neural network-based potential energy surfaces. Journal of Chemical Physics, 2020, 152, 214304.	3.0	21
31	Thermal activation of methane by MgO⁺: temperature dependent kinetics, reactive molecular dynamics simulations and statistical modeling. Physical Chemistry Chemical Physics, 2020, 22, 8913-8923.	2.8	12
32	Water Dynamics Around Proteins: T- and R-States of Hemoglobin and Melittin. Journal of Physical Chemistry B, 2020, 124, 6540-6554.	2.6	16
33	Non-conventional force fields for applications in spectroscopy and chemical reaction dynamics. Journal of Chemical Physics, 2020, 153, 010901.	3.0	20
34	High-dimensional potential energy surfaces for molecular simulations: from empiricism to machine learning. Machine Learning: Science and Technology, 2020, 1, 013001.	5.0	38
35	Formation and Stabilization of Ground and Excited-State Singlet O2 upon Recombination of 3P Oxygen on Amorphous Solid Water. Journal of Physical Chemistry Letters, 2020, 11, 2171-2176.	4.6	12
36	The N(⁴S) + O₂(X³Î£â^'g) â†" O(³P) + NO(X²Î) reaction: thermal and vibrational relaxation rates for the ²Aâ€², ⁴Aâ€² and ²Aâ€²â€² states. Physical Chemistry Chemical Physics, 2020, 22, 3927-3939.	2.8	30

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37	Dynamics and Infrared Spectrocopy of Monomeric and Dimeric Wild Type and Mutant Insulin. Journal of Physical Chemistry B, 2020, 124, 11882-11894.	2.6	13
38	Reactive dynamics and spectroscopy of hydrogen transfer from neural network-based reactive potential energy surfaces. New Journal of Physics, 2020, 22, 055002.	2.9	37
39	Reactive molecular dynamics: From small molecules to proteins. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1386.	14.6	37
40	Probing the Differential Dynamics of the Monomeric and Dimeric Insulin from Amide-I IR Spectroscopy. Journal of Physical Chemistry B, 2019, 123, 6588-6598.	2.6	10
41	Multistate Reactive Molecular Dynamics Simulations of Proton Diffusion in Water Clusters and in the Bulk. Journal of Physical Chemistry B, 2019, 123, 9846-9861.	2.6	12
42	Reactive atomistic simulations of Diels-Alder reactions: The importance of molecular rotations. Journal of Chemical Physics, 2019, 151, 104301.	3.0	23
43	Exhaustive state-to-state cross sections for reactive molecular collisions from importance sampling simulation and a neural network representation. Journal of Chemical Physics, 2019, 150, 211101.	3.0	35
44	PhysNet: A Neural Network for Predicting Energies, Forces, Dipole Moments, and Partial Charges. Journal of Chemical Theory and Computation, 2019, 15, 3678-3693.	5.3	501
45	Reactive molecular dynamics for the [Clâ€“CH₃â€“Br]^{â^’}reaction in the gas phase and in solution: a comparative study using empirical and neural network force fields. Electronic Structure, 2019, 1, 024002.	2.8	18
46	Vibrational Spectroscopy of N₃^{â€“} in the Gas and Condensed Phase. Journal of Physical Chemistry B, 2019, 123, 3282-3290.	2.6	18
47	O₂ formation in cold environments. Physical Chemistry Chemical Physics, 2019, 21, 6247-6255.	2.8	12
48	Sampling reactive regions in phase space by following the minimum dynamic path. Journal of Chemical Physics, 2019, 150, 074107.	3.0	9
49	Effect of Single-Point Mutations on Nitric Oxide Rebinding and the Thermodynamic Stability of Myoglobin. Journal of Physical Chemistry B, 2019, 123, 1961-1972.	2.6	2
50	Long-range versus short-range effects in cold molecular ion-neutral collisions. Nature Communications, 2019, 10, 5429.	12.8	53
51	Near dissociation states for H₂⁺â€“He on MRCI and FCI potential energy surfaces. Physical Chemistry Chemical Physics, 2019, 21, 24976-24983.	2.8	30
52	Molecular Determinants for Rate Acceleration in the Claisen Rearrangement Reaction. Journal of Physical Chemistry B, 2019, 123, 448-456.	2.6	14
53	Response to comment on 'Valid molecular dynamics simulations of human hemoglobin require a surprisingly large box size'. ELife, 2019, 8, .	6.0	13
54	Multi-State VALBOND for Atomistic Simulations of Hypervalent Molecules, Metal Complexes, and Reactions. Journal of Chemical Theory and Computation, 2018, 14, 3565-3578.	5.3	9

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55	Free energy simulations for protein ligand binding and stability. Molecular Simulation, 2018, 44, 1044-1061.	2.0	13
56	Kinetic Analysis and Structural Interpretation of Competitive Ligand Binding for NO Dioxygenation in Truncated Hemoglobinâ€...N. Angewandte Chemie - International Edition, 2018, 57, 3509-3513.	13.8	14
57	Solvent Composition Drives the Rebinding Kinetics of Nitric Oxide to Microperoxidase. Scientific Reports, 2018, 8, 5281.	3.3	4
58	Molecular Oxygen Formation in Interstellar Ices Does Not Require Tunneling. Journal of Physical Chemistry Letters, 2018, 9, 1822-1826.	4.6	15
59	A reactive, scalable, and transferable model for molecular energies from a neural network approach based on local information. Journal of Chemical Physics, 2018, 148, 241708.	3.0	74
60	The C(3P) + NO(X2Î) â†' O(3P) + CN(X2Î£+), N(2D)/N(4S) + CO(X1Î£+) reaction: Rates, branching ratios, and final states from 15 K to 20 000 K. Journal of Chemical Physics, 2018, 149, 094305.	3.0	43
61	The Role of Water in the Stability of Wild-type and Mutant Insulin Dimers. Journal of Physical Chemistry B, 2018, 122, 7038-7048.	2.6	23
62	An efficient water force field calibrated against intermolecular THz and Raman spectra. Journal of Chemical Physics, 2018, 148, 244504.	3.0	20
63	Valid molecular dynamics simulations of human hemoglobin require a surprisingly large box size. ELife, 2018, 7, .	6.0	63
64	From in silica to in silico: retention thermodynamics at solidâ€“liquid interfaces. Physical Chemistry Chemical Physics, 2018, 20, 18610-18622.	2.8	15
65	OH-Stretching Overtone Induced Dynamics in HSO₃F from Reactive Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2017, 121, 5079-5087.	2.5	13
66	Vibrational Stark spectroscopy for assessing ligand-binding strengths in a protein. Physical Chemistry Chemical Physics, 2017, 19, 16131-16143.	2.8	17
67	Communication: Vibrational relaxation of CO(1Î£) in collision with Ar(1S) at temperatures relevant to the hypersonic flight regime. Journal of Chemical Physics, 2017, 146, 111102.	3.0	6
68	Reactive collisions for NO(²Î) + N(⁴S) at temperatures relevant to the hypersonic flight regime. Physical Chemistry Chemical Physics, 2017, 19, 2392-2401.	2.8	29
69	Quantum and quasiclassical trajectory studies of rotational relaxation in Arâ€“N₂⁺ collisions. Physical Chemistry Chemical Physics, 2017, 19, 27945-27951.	2.8	2
70	Hydration Control Through Intramolecular Degrees of Freedom: Molecular Dynamics of [Cu(II)(Imidazole)₄]. Journal of Physical Chemistry B, 2017, 121, 9024-9031.	2.6	4
71	Molecular Mechanisms Underlying Solute Retention at Heterogeneous Interfaces. Journal of Physical Chemistry Letters, 2017, 8, 4600-4607.	4.6	26
72	Minimal distributed charges: Multipolar quality at the cost of point charge electrostatics. Journal of Chemical Physics, 2017, 147, 161712.	3.0	27

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73	Vibrational Spectroscopy and Proton Transfer Dynamics in Protonated Oxalate. Journal of Physical Chemistry A, 2017, 121, 5389-5398.	2.5	16
74	Toolkit for the Construction of Reproducing Kernel-Based Representations of Data: Application to Multidimensional Potential Energy Surfaces. Journal of Chemical Information and Modeling, 2017, 57, 1923-1931.	5.4	88
75	Perspective: THz-driven nuclear dynamics from solids to molecules. Structural Dynamics, 2017, 4, 061601.	2.3	22
76	Kinetic isotope effects and how to describe them. Structural Dynamics, 2017, 4, 061501.	2.3	37
77	Nonadiabatic effects in electronic and nuclear dynamics. Structural Dynamics, 2017, 4, 061510.	2.3	31
78	Ultrafast dynamics induced by the interaction of molecules with electromagnetic fields: Several quantum, semiclassical, and classical approaches. Structural Dynamics, 2017, 4, 061509.	2.3	3
79	Implications of short time scale dynamics on long time processes. Structural Dynamics, 2017, 4, 061507.	2.3	24
80	Migration of small ligands in globins: Xe diffusion in truncated hemoglobin N. PLoS Computational Biology, 2017, 13, e1005450.	3.2	4
81	Ligand and interfacial dynamics in a homodimeric hemoglobin. Structural Dynamics, 2016, 3, 012003.	2.3	6
82	Structure and Dynamics of Water/Methanol Mixtures at Hydroxylated Silica Interfaces Relevant to Chromatography. ChemPhysChem, 2016, 17, 2938-2944.	2.1	4
83	Collision-induced rotational excitation in N2+(2Î£g+,v=)â€“Ar: Comparison of computations and experiment. Journal of Chemical Physics, 2016, 144, 224307.	3.0	16
84	Impact of Quadrupolar Electrostatics on Atoms Adjacent to the Sigma-Hole in Condensed-Phase Simulations. Journal of Chemical Theory and Computation, 2016, 12, 3008-3019.	5.3	23
85	Spectroscopy and dynamics of double proton transfer in formic acid dimer. Physical Chemistry Chemical Physics, 2016, 18, 24654-24662.	2.8	44
86	Extending Halogen-based Medicinal Chemistry to Proteins. Journal of Biological Chemistry, 2016, 291, 27023-27041.	3.4	25
87	A Toolkit to Fit Nonbonded Parameters from and for Condensed Phase Simulations. Journal of Chemical Information and Modeling, 2016, 56, 1479-1489.	5.4	25
88	Strukturelle Interpretation metastabiler ZustÃnde in Myoglobinâ€NO. Angewandte Chemie, 2016, 128, 10280-10285.	2.0	2
89	Structural Interpretation of Metastable States in Myoglobinâ€“NO. Angewandte Chemie - International Edition, 2016, 55, 10126-10130.	13.8	28
90	Inner-Shell Water Rearrangement Following Photoexcitation of Tris(2,2â€²-bipyridine)iron(II). Journal of Physical Chemistry B, 2016, 120, 206-216.	2.6	21

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91	Copper Oxidation/Reduction in Water and Protein: Studies with DFTB3/MM and VALBOND Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2016, 120, 1894-1910.	2.6	22
92	Sequential Proton Coupled Electron Transfer (PCET): Dynamics Observed over 8 Orders of Magnitude in Time. Journal of the American Chemical Society, 2016, 138, 4401-4407.	13.7	21
93	HSO₃Cl: a prototype molecule for studying OH-stretching overtone induced photodissociation. Physical Chemistry Chemical Physics, 2016, 18, 6780-6788.	2.8	15
94	Charge Transfer Pathways in Three Isomers of Naphthalene-Bridged Organic Mixed Valence Compounds. Journal of Organic Chemistry, 2016, 81, 595-602.	3.2	34
95	Reproducing kernel potential energy surfaces in biomolecular simulations: Nitric oxide binding to myoglobin. Journal of Chemical Physics, 2015, 143, 105103.	3.0	16
96	Communication: Equilibrium rate coefficients from atomistic simulations: The O(3P) + NO(2Î) â†' O2(X3Î£gâ^) + N(4S) reaction at temperatures relevant to the hypersonic flight regime. Journal of Chemical Physics, 2015, 142, 091104.	3.0	22
97	Following the molecular motion of near-resonant excited CO on Pt(111): A simulated x-ray photoelectron diffraction study based on molecular dynamics calculations. Structural Dynamics, 2015, 2, 035102.	2.3	6
98	Coupled proteinâ€"ligand dynamics in truncated hemoglobin N from atomistic simulations and transition networks. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 996-1005.	2.4	9
99	Vibrational Relaxation and Energy Migration of N-Methylacetamide in Water: The Role of Nonbonded Interactions. Journal of Physical Chemistry B, 2015, 119, 3112-3122.	2.6	11
100	Infrared and Near-Infrared Spectroscopy of Acetylacetone and Hexafluoroacetylacetone. Journal of Physical Chemistry A, 2015, 119, 7980-7990.	2.5	43
101	A comparative analysis of clustering algorithms: O2 migration in truncated hemoglobin I from transition networks. Journal of Chemical Physics, 2015, 142, 025103.	3.0	10
102	Solvation of fluoro-acetonitrile in water by 2D-IR spectroscopy: A combined experimental-computational study. Journal of Chemical Physics, 2015, 142, 212415.	3.0	13
103	The effect of classical and quantum dynamics on vibrational frequency shifts of H2 in clathrate hydrates. Journal of Chemical Physics, 2014, 140, 024311.	3.0	10
104	Computational study of collisions between O(3P) and NO(2Î) at temperatures relevant to the hypersonic flight regime. Journal of Chemical Physics, 2014, 141, 164319.	3.0	34
105	Spatial Averaging: Sampling Enhancement for Exploring Configurational Space of Atomic Clusters and Biomolecules. Journal of Chemical Theory and Computation, 2014, 10, 4284-4296.	5.3	1
106	A supervised fitting approach to force field parametrization with application to the SIBFA polarizable force field. Journal of Computational Chemistry, 2014, 35, 1577-1591.	3.3	21
107	CO-dynamics in the active site of cytochrome c oxidase. Journal of Chemical Physics, 2014, 140, 145101.	3.0	6
108	Computational Analysis of Methyl Transfer Reactions in Dengue Virus Methyltransferase. Journal of Physical Chemistry B, 2014, 118, 5882-5890.	2.6	11

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109	Diffusion of atomic oxygen relevant to water formation in amorphous interstellar ices. Faraday Discussions, 2014, 168, 205-222.	3.2	13
110	Multisurface Adiabatic Reactive Molecular Dynamics. Journal of Chemical Theory and Computation, 2014, 10, 1366-1375.	5.3	60
111	Kinetic isotope effect in malonaldehyde determined from path integral Monte Carlo simulations. Physical Chemistry Chemical Physics, 2014, 16, 204-211.	2.8	35
112	Competitive reaction pathways in vibrationally induced photodissociation of H₂SO₄. Physical Chemistry Chemical Physics, 2014, 16, 18533.	2.8	17
113	Computational Two-Dimensional Infrared Spectroscopy without Maps: N-Methylacetamide in Water. Journal of Physical Chemistry B, 2014, 118, 8135-8147.	2.6	27
114	A Novel, Computationally Efficient Multipolar Model Employing Distributed Charges for Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 4229-4241.	5.3	31
115	Quantitative Atomistic Simulations of Reactive and Non-Reactive Processes. Chimia, 2014, 68, 592.	0.6	0
116	Overcoming the Rare Event Sampling Problem in Biological Systems with Infinite Swapping. Journal of Chemical Theory and Computation, 2013, 9, 4215-4224.	5.3	21
117	Multipole-Based Force Fields from ab Initio Interaction Energies and the Need for Jointly Refitting All Intermolecular Parameters. Journal of Chemical Theory and Computation, 2013, 9, 1499-1511.	5.3	35
118	Deriving Static Atomic Multipoles from the Electrostatic Potential. Journal of Chemical Information and Modeling, 2013, 53, 3410-3417.	5.4	25
119	Structure and dynamics of solvent shells around photoexcited metal complexes. Physical Chemistry Chemical Physics, 2013, 15, 6268.	2.8	17
120	Reactionâ€Pathway Selection in the Structural Dynamics of a Heme Protein. Chemistry - A European Journal, 2013, 19, 3558-3562.	3.3	13
121	Scoring Multipole Electrostatics in Condensed-Phase Atomistic Simulations. Journal of Physical Chemistry B, 2013, 117, 5460-5471.	2.6	18
122	Hydration free energies of cyanide and hydroxide ions from molecular dynamics simulations with accurate force fields. Physical Chemistry Chemical Physics, 2013, 15, 20303.	2.8	19
123	Toward a Broadly Applicable Force Field for d⁶-Piano Stool Complexes. Journal of Chemical Theory and Computation, 2013, 9, 2313-2323.	5.3	6
124	Leveraging Symmetries of Static Atomic Multipole Electrostatics in Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 5450-5459.	5.3	49
125	2D IR spectra of cyanide in water investigated by molecular dynamics simulations. Journal of Chemical Physics, 2013, 139, 054506.	3.0	53
126	Oxygen Migration Pathways in NOâ€bound Truncated Hemoglobin. ChemPhysChem, 2012, 13, 4276-4286.	2.1	22

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127	Arylsulfonamides as inhibitors for carbonic anhydrase: prediction & validation. Chemical Science, 2012, 3, 690-700.	7.4	20
128	Dynamics of Water/Methanol Mixtures at Functionalized Chromatographic Interfaces. Journal of Physical Chemistry B, 2012, 116, 10951-10959.	2.6	21
129	Temperature Dependence of the Heat Diffusivity of Proteins. Journal of Physical Chemistry A, 2012, 116, 2620-2628.	2.5	27
130	State-selected ionâ€“molecule reactions with Coulomb-crystallized molecular ions in traps. Chemical Physics Letters, 2012, 547, 1-8.	2.6	39
131	Hydrogen-Bond and Solvent Dynamics in Transition Metal Complexes: A Combined Simulation and NMR-Investigation. Journal of Physical Chemistry B, 2012, 116, 14406-14415.	2.6	16
132	Atomistic simulations of reactive processes in the gas- and condensed-phase. International Reviews in Physical Chemistry, 2012, 31, 235-264.	2.3	4
133	Atomic multipoles: Electrostatic potential fit, local reference axis systems, and conformational dependence. Journal of Computational Chemistry, 2012, 33, 1673-1688.	3.3	56
134	Reaction Dynamics: Rules Change with Molecular Size. ChemPhysChem, 2012, 13, 684-685.	2.1	0
135	On the Role of Nonbonded Interactions in Vibrational Energy Relaxation of Cyanide in Water. Journal of Physical Chemistry A, 2011, 115, 5053-5061.	2.5	40
136	Vibrationally Induced Dissociation of Sulfuric Acid (H₂SO₄). Journal of Physical Chemistry A, 2011, 115, 14350-14360.	2.5	25
137	Water-assisted Proton Transfer in Ferredoxin I. Journal of Biological Chemistry, 2011, 286, 23679-23687.	3.4	14
138	Theoretical and Computational Chemistry. Chimia, 2010, 64, 867.	0.6	0
139	Finite-temperature quantum simulations of mixed rare gas clusters. Journal of Chemical Physics, 2010, 132, 234315.	3.0	1
140	A generalized reactive force field for nonlinear hydrogen bonds: Hydrogen dynamics and transfer in malonaldehyde. Journal of Chemical Physics, 2010, 133, 064503.	3.0	42
141	Spatial averaging for small molecule diffusion in condensed phase environments. Journal of Chemical Physics, 2010, 133, 044506.	3.0	7
142	Explicit Hydrogen-Bond Potentials and Their Application to NMR Scalar Couplings in Proteins. Journal of Chemical Theory and Computation, 2010, 6, 467-476.	5.3	16
143	Dynamics of Water Filaments in Disordered Environments. Journal of Physical Chemistry B, 2010, 114, 12203-12212.	2.6	12
144	Higher order multipole moments for molecular dynamics simulations. Journal of Molecular Modeling, 2009, 15, 687-694.	1.8	19

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145	Application of Multipolar Charge Models and Molecular Dynamics Simulations to Study Stark Shifts in Inhomogeneous Electric Fields. Journal of Physical Chemistry A, 2009, 113, 13199-13209.	2.5	22
146	Molecular Mechanics Force Field for Octahedral Organometallic Compounds with Inclusion of the Trans Influence. Journal of Chemical Theory and Computation, 2009, 5, 530-539.	5.3	36
147	Atomistic Simulations of CO Vibrations in Ices Relevant to Astrochemistry. ChemPhysChem, 2008, 9, 1271-1277.	2.1	17
148	Reactive force fields for proton transfer dynamics. Journal of Computational Chemistry, 2008, 29, 1048-1063.	3.3	47
149	The Role of Higher CO-Multipole Moments in Understanding the Dynamics of Photodissociated Carbonmonoxide in Myoglobin. Biophysical Journal, 2008, 94, 2505-2515.	0.5	73
150	Solvent structures of mixed water/acetonitrile mixtures at chromatographic interfaces from computer simulations. Physical Chemistry Chemical Physics, 2008, 10, 4765.	2.8	40
151	Counterion effect on the formation of coordination polymer networks between AgNO3 and L (2,2â€²-oxybis(ethane-2,1-diyl) diisonicotinate). Part 2. CrystEngComm, 2008, 10, 1542.	2.6	33
152	Atomistic Simulation of Adiabatic Reactive Processes Based on Multi-State Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2008, 4, 1083-1093.	5.3	65
153	Direct Comparison of Experimental and Calculated NMR Scalar Coupling Constants for Force Field Validation and Adaptation. Journal of Chemical Theory and Computation, 2008, 4, 1949-1958.	5.3	9
154	MD simulations using distributed multipole electrostatics: Structural and spectroscopic properties of CO- and methane-containing clathrates. Molecular Physics, 2008, 106, 1675-1684.	1.7	18
155	Diffusive dynamics on multidimensional rough free energy surfaces. Journal of Chemical Physics, 2007, 127, 135101.	3.0	26
156	Investigating the Relationship between Infrared Spectra of Shared Protons in Different Chemical Environments:Â A Comparison of Protonated Diglyme and Protonated Water Dimer. Journal of Physical Chemistry A, 2007, 111, 1638-1647.	2.5	26
157	Energetics and Dynamics in MbCN:Â CN--Vibrational Relaxation from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 218-226.	2.6	17
158	Adsorption of Acridine Orange at a C8,18/Water/Acetonitrile Interface. Journal of Physical Chemistry B, 2007, 111, 10208-10216.	2.6	41
159	Computer simulations of structures, energetics and dynamics of myoglobinâ€‰Â·Â·Â·â€‰ligand complexes. International Reviews in Physical Chemistry, 2006, 25, 407-425.	2.3	11
160	Studying Reactive Processes with Classical Dynamics: Rebinding Dynamics in MbNO. Biophysical Journal, 2006, 90, 1191-1201.	0.5	65
161	How inaccuracies in protein structure models affect estimates of protein-ligand interactions: Computational analysis of HIV-I protease inhibitor binding. Proteins: Structure, Function and Bioinformatics, 2006, 65, 407-423.	2.6	28
162	Importance of individual side chains for the stability of a protein fold: Computational alanine scanning of the insulin monomer. Journal of Computational Chemistry, 2006, 27, 1843-1857.	3.3	45

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163	On the Influence of the Local Environment on the CO Stretching Frequencies in Native Myoglobin: Assignment of the B-States in MbCO. ChemPhysChem, 2006, 7, 2061-2063.	2.1	42
164	Study of the insulin dimerization: Binding free energy calculations and per-residue free energy decomposition. Proteins: Structure, Function and Bioinformatics, 2005, 61, 79-93.	2.6	202
165	Free-Energy Barriers in MbCO Rebinding. Journal of Physical Chemistry B, 2005, 109, 16911-16917.	2.6	40
166	Hierarchical Numerical Solution of Smoluchowski Equations with Rough Potentials. Journal of Chemical Theory and Computation, 2005, 1, 208-214.	5.3	9
167	Potential Energy Surface and Molecular Dynamics of MbNO:Â Existence of an Unsuspected FeON Minimum. Journal of Physical Chemistry B, 2005, 109, 21118-21125.	2.6	32
168	CO migration in native and mutant myoglobin: Atomistic simulations for the understanding of protein function. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 5998-6002.	7.1	91
169	Ligand Dynamics in Myoglobin: Calculation of Infrared Spectra for Photodissociated NO. ChemPhysChem, 2004, 5, 1710-1718.	2.1	26
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