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	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
2	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
3	Machine Learning for Chemical Reactions. Chemical Reviews, 2021, 121, 10218-10239.	47.7	166
4	Morphing ab initio potentials: A systematic study of Neâ€“HF. Journal of Chemical Physics, 1999, 110, 8338-8347.	3.0	131
5	NO rebinding to myoglobin: a reactive molecular dynamics study. Biophysical Chemistry, 2002, 98, 183-207.	2.8	107
6	Theoretical Investigation of Infrared Spectra and Pocket Dynamics of Photodissociated Carbonmonoxy Myoglobin. Biophysical Journal, 2003, 85, 3612-3623.	0.5	98
7	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
8	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
9	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
10	Double proton transfer in the isolated and DNA-embedded guanine-cytosine base pair. Journal of Chemical Physics, 2004, 121, 4377-4388.	3.0	73
11	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
12	Simulation of proton transfer along ammonia wires: An â€œab initioâ€•and semiempirical density functional comparison of potentials and classical molecular dynamics. Journal of Chemical Physics, 2002, 116, 2572-2585.	3.0	72
13	A Comparison of the Dynamic Behavior of Monomeric and Dimeric Insulin Shows Structural Rearrangements in the Active Monomer. Journal of Molecular Biology, 2004, 342, 913-929.	4.2	68
14	Studying Reactive Processes with Classical Dynamics: Rebinding Dynamics in MbNO. Biophysical Journal, 2006, 90, 1191-1201.	0.5	65
15	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
16	Valid molecular dynamics simulations of human hemoglobin require a surprisingly large box size. ELife, 2018, 7, .	6.0	63
17	Multisurface Adiabatic Reactive Molecular Dynamics. Journal of Chemical Theory and Computation, 2014, 10, 1366-1375.	5.3	60
18	Atomic multipoles: Electrostatic potential fit, local reference axis systems, and conformational dependence. Journal of Computational Chemistry, 2012, 33, 1673-1688.	3.3	56

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19	2D IR spectra of cyanide in water investigated by molecular dynamics simulations. Journal of Chemical Physics, 2013, 139, 054506.	3.0	53
20	Long-range versus short-range effects in cold molecular ion-neutral collisions. Nature Communications, 2019, 10, 5429.	12.8	53
21	Leveraging Symmetries of Static Atomic Multipole Electrostatics in Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 5450-5459.	5.3	49
22	Reactive force fields for proton transfer dynamics. Journal of Computational Chemistry, 2008, 29, 1048-1063.	3.3	47
23	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
24	The potential energy surface and near-dissociation states of He-H2+. Journal of Chemical Physics, 1999, 110, 3418-3427.	3.0	44
25	Spectroscopy and dynamics of double proton transfer in formic acid dimer. Physical Chemistry Chemical Physics, 2016, 18, 24654-24662.	2.8	44
26	Infrared and Near-Infrared Spectroscopy of Acetylacetone and Hexafluoroacetylacetone. Journal of Physical Chemistry A, 2015, 119, 7980-7990.	2.5	43
27	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
28	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
29	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
30	Adsorption of Acridine Orange at a C8,18/Water/Acetonitrile Interface. Journal of Physical Chemistry B, 2007, 111, 10208-10216.	2.6	41
31	Free-Energy Barriers in MbCO Rebinding. Journal of Physical Chemistry B, 2005, 109, 16911-16917.	2.6	40
32	Solvent structures of mixed water/acetonitrile mixtures at chromatographic interfaces from computer simulations. Physical Chemistry Chemical Physics, 2008, 10, 4765.	2.8	40
33	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
34	State-selected ionâ€“molecule reactions with Coulomb-crystallized molecular ions in traps. Chemical Physics Letters, 2012, 547, 1-8.	2.6	39
35	High-dimensional potential energy surfaces for molecular simulations: from empiricism to machine learning. Machine Learning: Science and Technology, 2020, 1, 013001.	5.0	38
36	Kinetic isotope effects and how to describe them. Structural Dynamics, 2017, 4, 061501.	2.3	37

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37	Reactive molecular dynamics: From small molecules to proteins. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1386.	14.6	37
38	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
39	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
40	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
41	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
42	Kinetic isotope effect in malonaldehyde determined from path integral Monte Carlo simulations. Physical Chemistry Chemical Physics, 2014, 16, 204-211.	2.8	35
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	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
45	Charge Transfer Pathways in Three Isomers of Naphthalene-Bridged Organic Mixed Valence Compounds. Journal of Organic Chemistry, 2016, 81, 595-602.	3.2	34
46	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
47	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
48	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
49	Nonadiabatic effects in electronic and nuclear dynamics. Structural Dynamics, 2017, 4, 061510.	2.3	31
50	How many structures are there for {[AgL](NO3)(H2O)n}? Water-content dependent variations in the structure of {[AgL](NO3)(H2O)n}, n= 0, 1, 2; L = ethanediyl bis(isonicotinate). CrystEngComm, 2004, 6, 336.	2.6	30
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	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
53	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
54	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

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55	Structural Interpretation of Metastable States in Myoglobinâ€“NO. Angewandte Chemie - International Edition, 2016, 55, 10126-10130.	13.8	28
56	Temperature Dependence of the Heat Diffusivity of Proteins. Journal of Physical Chemistry A, 2012, 116, 2620-2628.	2.5	27
57	Computational Two-Dimensional Infrared Spectroscopy without Maps: N-Methylacetamide in Water. Journal of Physical Chemistry B, 2014, 118, 8135-8147.	2.6	27
58	Minimal distributed charges: Multipolar quality at the cost of point charge electrostatics. Journal of Chemical Physics, 2017, 147, 161712.	3.0	27
59	Ligand Dynamics in Myoglobin: Calculation of Infrared Spectra for Photodissociated NO. ChemPhysChem, 2004, 5, 1710-1718.	2.1	26
60	Diffusive dynamics on multidimensional rough free energy surfaces. Journal of Chemical Physics, 2007, 127, 135101.	3.0	26
61	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
62	Molecular Mechanisms Underlying Solute Retention at Heterogeneous Interfaces. Journal of Physical Chemistry Letters, 2017, 8, 4600-4607.	4.6	26
63	Intermolecular potential energy surfaces and bound states in Fâ€“HF. Journal of Chemical Physics, 2000, 112, 592-600.	3.0	25
64	Vibrationally Induced Dissociation of Sulfuric Acid (H₂SO₄). Journal of Physical Chemistry A, 2011, 115, 14350-14360.	2.5	25
65	Deriving Static Atomic Multipoles from the Electrostatic Potential. Journal of Chemical Information and Modeling, 2013, 53, 3410-3417.	5.4	25
66	Extending Halogen-based Medicinal Chemistry to Proteins. Journal of Biological Chemistry, 2016, 291, 27023-27041.	3.4	25
67	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
68	Implications of short time scale dynamics on long time processes. Structural Dynamics, 2017, 4, 061507.	2.3	24
69	Machine Learning Models of Vibrating H₂CO: Comparing Reproducing Kernels, FCHL, and PhysNet. Journal of Physical Chemistry A, 2020, 124, 8853-8865.	2.5	24
70	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
71	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
72	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

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73	Reactive atomistic simulations of Diels-Alder reactions: The importance of molecular rotations. Journal of Chemical Physics, 2019, 151, 104301.	3.0	23
74	Potential energy surfaces and bound states for the open-shell van der Waals cluster Brâ€“HF. Journal of Chemical Physics, 2003, 119, 8873-8881.	3.0	22
75	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
76	Oxygen Migration Pathways in NOâ€bound Truncated Hemoglobin. ChemPhysChem, 2012, 13, 4276-4286.	2.1	22
77	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
78	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
79	Perspective: THz-driven nuclear dynamics from solids to molecules. Structural Dynamics, 2017, 4, 061601.	2.3	22
80	Dynamics of Water/Methanol Mixtures at Functionalized Chromatographic Interfaces. Journal of Physical Chemistry B, 2012, 116, 10951-10959.	2.6	21
81	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
82	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
83	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
84	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
85	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
86	Arylsulfonamides as inhibitors for carbonic anhydrase: prediction & validation. Chemical Science, 2012, 3, 690-700.	7.4	20
87	An efficient water force field calibrated against intermolecular THz and Raman spectra. Journal of Chemical Physics, 2018, 148, 244504.	3.0	20
88	Non-conventional force fields for applications in spectroscopy and chemical reaction dynamics. Journal of Chemical Physics, 2020, 153, 010901.	3.0	20
89	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
90	Potential energy surfaces and properties of the Brâ€“HBr complex. Physical Chemistry Chemical Physics, 2000, 2, 441-446.	2.8	19

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91	Higher order multipole moments for molecular dynamics simulations. Journal of Molecular Modeling, 2009, 15, 687-694.	1.8	19
92	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
93	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
94	Scoring Multipole Electrostatics in Condensed-Phase Atomistic Simulations. Journal of Physical Chemistry B, 2013, 117, 5460-5471.	2.6	18
95	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
96	Vibrational Spectroscopy of N₃^{â€“} in the Gas and Condensed Phase. Journal of Physical Chemistry B, 2019, 123, 3282-3290.	2.6	18
97	Structures and energetics of Neâ€“HN2+ clusters. Journal of Chemical Physics, 1999, 111, 2633-2640.	3.0	17
98	Theoretical Investigations on Azotobacter vinelandii Ferredoxin I: Effects of Electron Transfer on Protein Dynamics. Biophysical Journal, 2004, 86, 1987-2007.	0.5	17
99	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
100	Atomistic Simulations of CO Vibrations in Ices Relevant to Astrochemistry. ChemPhysChem, 2008, 9, 1271-1277.	2.1	17
101	Structure and dynamics of solvent shells around photoexcited metal complexes. Physical Chemistry Chemical Physics, 2013, 15, 6268.	2.8	17
102	Competitive reaction pathways in vibrationally induced photodissociation of H₂SO₄. Physical Chemistry Chemical Physics, 2014, 16, 18533.	2.8	17
103	Vibrational Stark spectroscopy for assessing ligand-binding strengths in a protein. Physical Chemistry Chemical Physics, 2017, 19, 16131-16143.	2.8	17
104	The potential energy surface and rovibrational states of Heâ€“HCO+. Journal of Chemical Physics, 1999, 110, 4347-4353.	3.0	16
105	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
106	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
107	Reproducing kernel potential energy surfaces in biomolecular simulations: Nitric oxide binding to myoglobin. Journal of Chemical Physics, 2015, 143, 105103.	3.0	16
108	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

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109	Vibrational Spectroscopy and Proton Transfer Dynamics in Protonated Oxalate. Journal of Physical Chemistry A, 2017, 121, 5389-5398.	2.5	16
110	Water Dynamics Around Proteins: T- and R-States of Hemoglobin and Melittin. Journal of Physical Chemistry B, 2020, 124, 6540-6554.	2.6	16
111	HSO₃Cl: a prototype molecule for studying OH-stretching overtone induced photodissociation. Physical Chemistry Chemical Physics, 2016, 18, 6780-6788.	2.8	15
112	Molecular Oxygen Formation in Interstellar Ices Does Not Require Tunneling. Journal of Physical Chemistry Letters, 2018, 9, 1822-1826.	4.6	15
113	From in silica to in silico: retention thermodynamics at solidâ€“liquid interfaces. Physical Chemistry Chemical Physics, 2018, 20, 18610-18622.	2.8	15
114	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
115	Theoretical investigations of Ferredoxin I: The possible role of internal water molecules on the coupled electron proton transfer reaction. Faraday Discussions, 2003, 124, 297.	3.2	14
116	Water-assisted Proton Transfer in Ferredoxin I. Journal of Biological Chemistry, 2011, 286, 23679-23687.	3.4	14
117	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
118	Molecular Determinants for Rate Acceleration in the Claisen Rearrangement Reaction. Journal of Physical Chemistry B, 2019, 123, 448-456.	2.6	14
119	Reactionâ€Pathway Selection in the Structural Dynamics of a Heme Protein. Chemistry - A European Journal, 2013, 19, 3558-3562.	3.3	13
120	Diffusion of atomic oxygen relevant to water formation in amorphous interstellar ices. Faraday Discussions, 2014, 168, 205-222.	3.2	13
121	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
122	OH-Stretching Overtone Induced Dynamics in HSO₃F from Reactive Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2017, 121, 5079-5087.	2.5	13
123	Free energy simulations for protein ligand binding and stability. Molecular Simulation, 2018, 44, 1044-1061.	2.0	13
124	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
125	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
126	Response to comment on 'Valid molecular dynamics simulations of human hemoglobin require a surprisingly large box size'. ELife, 2019, 8, .	6.0	13

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127	Dynamics of Water Filaments in Disordered Environments. Journal of Physical Chemistry B, 2010, 114, 12203-12212.	2.6	12
128	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
129	O₂ formation in cold environments. Physical Chemistry Chemical Physics, 2019, 21, 6247-6255.	2.8	12
130	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
131	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
132	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
133	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
134	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
135	Computational Analysis of Methyl Transfer Reactions in Dengue Virus Methyltransferase. Journal of Physical Chemistry B, 2014, 118, 5882-5890.	2.6	11
136	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
137	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
138	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
139	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
140	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
141	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
142	Hierarchical Numerical Solution of Smoluchowski Equations with Rough Potentials. Journal of Chemical Theory and Computation, 2005, 1, 208-214.	5.3	9
143	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
144	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

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145	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
146	Sampling reactive regions in phase space by following the minimum dynamic path. Journal of Chemical Physics, 2019, 150, 074107.	3.0	9
147	Polarizable Multipolar Molecular Dynamics Using Distributed Point Charges. Journal of Chemical Theory and Computation, 2020, 16, 7267-7280.	5.3	8
148	Site-selective dynamics of azidolysozyme. Journal of Chemical Physics, 2021, 154, 165101.	3.0	8
149	Thermal and Vibrationally Activated Decomposition of the syn-CH₃CHOO Criegee Intermediate. ACS Earth and Space Chemistry, 2021, 5, 3396-3406.	2.7	8
150	Solvent Effects on the Menshutkin Reaction. Journal of Physical Chemistry B, 2022, 126, 1951-1961.	2.6	8
151	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
152	Spatial averaging for small molecule diffusion in condensed phase environments. Journal of Chemical Physics, 2010, 133, 044506.	3.0	7
153	N3+: Full-dimensional ground state potential energy surface, vibrational energy levels, and dynamics. Journal of Chemical Physics, 2020, 153, 044302.	3.0	7
154	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
155	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
156	The Potential Energy Surface and Ro-Vibrational States of Heâ”CH+. Journal of Physical Chemistry A, 2000, 104, 1271-1277.	2.5	6
157	Toward a Broadly Applicable Force Field for d⁶-Piano Stool Complexes. Journal of Chemical Theory and Computation, 2013, 9, 2313-2323.	5.3	6
158	CO-dynamics in the active site of cytochrome c oxidase. Journal of Chemical Physics, 2014, 140, 145101.	3.0	6
159	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
160	Ligand and interfacial dynamics in a homodimeric hemoglobin. Structural Dynamics, 2016, 3, 012003.	2.3	6
161	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
162	Spectroscopy, Dynamics, and Hydration of S-Nitrosylated Myoglobin. Journal of Physical Chemistry B, 2021, 125, 4262-4273.	2.6	6

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163	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
164	Energy Redistribution Following CO2 Formation on Cold Amorphous Solid Water. Frontiers in Chemistry, 2021, 9, 827085.	3.6	6
165	Mechanistic Insight into the Precursor Chemistry of ZrO₂and HfO₂Nanocrystals; towards Size-Tunable Syntheses. Jacs Au, 2022, 2, 827-838.	7.9	6
166	Quantum Simulations of Nenâ”'OH+ Clusters. Journal of Physical Chemistry A, 2000, 104, 7144-7150.	2.5	5
167	Atomistic simulations of reactive processes in the gas- and condensed-phase. International Reviews in Physical Chemistry, 2012, 31, 235-264.	2.3	4
168	Structure and Dynamics of Water/Methanol Mixtures at Hydroxylated Silica Interfaces Relevant to Chromatography. ChemPhysChem, 2016, 17, 2938-2944.	2.1	4
169	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
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