Philipp Marquetand

List of Publications by Year
in descending order

100 papers	6,090 citations	109137 35 h-index	71532 76 g-index
106 all docs	106 docs citations	106 times ranked	5122 citing authors

#	Article	IF	Citations
1	BuRNN: Buffer Region Neural Network Approach for Polarizable-Embedding Neural Network/Molecular Mechanics Simulations. Journal of Physical Chemistry Letters, 2022, 13, 3812-3818.	2.1	18
2	Solving the electronic SchrÃ¶dinger equation for multiple nuclear geometries with weight-sharing deep neural networks. Nature Computational Science, 2022, 2, 331-341.	3.8	25
3	Deep learning study of tyrosine reveals that roaming can lead to photodamage. Nature Chemistry, 2022, 14, 914-919.	6.6	21
4	Machine Learning for Electronically Excited States of Molecules. Chemical Reviews, 2021, 121, 9873-9926.	23.0	207
5	Ultrafast photochemistry of a molybdenum carbonylâ€“nitrosyl complex with a triazacyclononane coligand. Physical Chemistry Chemical Physics, 2021, 23, 24187-24199.	1.3	2
6	Competition between dynamic resonance and internal conversion in strong-field molecular ionization with chirped ultrafast laser pulses. Physical Review A, 2021, 103, .	1.0	8
7	Development of a Hybrid Neural Network/Molecular Mechanics Approach for Metalloprotein Simulations. Biophysical Journal, 2021, 120, 195a.	0.2	0
8	A Force Field for a Manganese-Vanadium Water Oxidation Catalyst: Redox Potentials in Solution as Showcase. Catalysts, 2021, 11, 493.	1.6	8
9	Tridentate 3-Substituted Naphthoquinone Ruthenium Arene Complexes: Synthesis, Characterization, Aqueous Behavior, and Theoretical and Biological Studies. Inorganic Chemistry, 2021, 60, 9805-9819.	1.9	9
10	Photoâ€Initiated Cobaltâ€Catalyzed Radical Olefin Hydrogenation. Chemistry - A European Journal, 2021, 27, 16978-16989.	1.7	8
11	Femtosecond molecular dynamics viewed by multi-model imaging. , 2021, , .		0
12	Activation by oxidation and ligand exchange in a molecular manganese vanadium oxide water oxidation catalyst. Chemical Science, 2021, 12, 12918-12927.	3.7	10
13	Coherent Control of Internal Conversion in Strong-Field Molecular Ionization. Physical Review Letters, 2020, 125, 053202.	2.9	10
14	Deep learning for UV absorption spectra with SchNarc: First steps toward transferability in chemical compound space. Journal of Chemical Physics, 2020, 153, 154112.	1.2	50
15	Excited-state dynamics of CH2I2 and CH2IBr studied with UV-pump VUV-probe momentum-resolved photoion spectroscopy. Journal of Chemical Physics, 2020, 153, 184304.	1.2	9
16	Neural networks and kernel ridge regression for excited states dynamics of CH₂NH 2+ : From single-state to multi-state representations and multi-property machine learning models. Machine Learning: Science and Technology, 2020, 1, 025009.	2.4	47
17	Combining SchNet and SHARC: The SchNarc Machine Learning Approach for Excited-State Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 3828-3834.	2.1	114
18	Spectroscopic and Structural Probing of Excited-State Molecular Dynamics with Time-Resolved Photoelectron Spectroscopy and Ultrafast Electron Diffraction. Physical Review X, 2020, 10, .	2.8	11

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19	Molecular Dynamics with Neural Network Potentials. Lecture Notes in Physics, 2020, , 233-252.	0.3	12
20	Machine Learning for Nonadiabatic Molecular Dynamics. RSC Theoretical and Computational Chemistry Series, 2020, , 76-108.	0.7	3
21	Machine learning and excited-state molecular dynamics. Machine Learning: Science and Technology, 2020, 1, 043001.	2.4	50
22	Adiabatic elimination in strong-field light-matter coupling. Physical Review A, 2020, 102, .	1.0	11
23	Machine learning enables long time scale molecular photodynamics simulations. Chemical Science, 2019, 10, 8100-8107.	3.7	140
24	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661
25	Excited state dynamics of CH2I2 and CH2BrI studied with UV pump VUV probe photoelectron spectroscopy. Journal of Chemical Physics, 2019, 150, 174201.	1.2	23
26	Exploring density functional subspaces with genetic algorithms. Monatshefte FÃ¼r Chemie, 2019, 150, 173-182.	0.9	8
27	wACSFâ€"Weighted atom-centered symmetry functions as descriptors in machine learning potentials. Journal of Chemical Physics, 2018, 148, 241709.	1.2	198
28	Machine Learning for Organic Synthesis: Are Robots Replacing Chemists?. Angewandte Chemie - International Edition, 2018, 57, 6978-6980.	7.2	56
29	Stepwise photosensitized thymine dimerization mediated by an exciton intermediate. Monatshefte FÃ¼r Chemie, 2018, 149, 1-9.	0.9	14
30	Strong-field- versus weak-field-ionization pump-probe spectroscopy. Physical Review A, 2018, 98, .	1.0	16
31	Simulated and Experimental Time-Resolved Photoelectron Spectra of the Intersystem Crossing Dynamics in 2-Thiouracil. Molecules, 2018, 23, 2836.	1.7	28
32	Cover Image, Volume 8, Issue 6. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1400.	6.2	7
33	Nonadiabatic dynamics: The SHARC approach. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1370.	6.2	274
34	Maschinelles Lernen fÃ¼r die organische Synthese: Ersetzen Roboter Chemiker?. Angewandte Chemie, 2018, 130, 7096-7098.	1.6	8
35	General Trajectory Surface Hopping Method for Ultrafast Nonadiabatic Dynamics. RSC Theoretical and Computational Chemistry Series, 2018, , 348-385.	0.7	3
36	Ab initio molecular dynamics relaxation and intersystem crossing mechanisms of 5-azacytosine. Physical Chemistry Chemical Physics, 2017, 19, 5888-5894.	1.3	31

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37	Solvatochromic Effects on the Absorption Spectrum of 2-Thiocytosine. Journal of Physical Chemistry B, 2017, 121, 5187-5196.	1.2	31
38	2-Thiouracil intersystem crossing photodynamics studied by wavelength-dependent photoelectron and transient absorption spectroscopies. Physical Chemistry Chemical Physics, 2017, 19, 19756-19766.	1.3	58
39	Publisher's Note: Molecular oxygen observed by direct photoproduction from carbon dioxide [Phys. Rev. A 95 , 011404(R) (2017)]. Physical Review A, 2017, 95, .	1.0	2
40	Ionic dynamics underlying strong-field dissociative molecular ionization. Physical Review A, 2017, 96, .	1.0	3
41	Molecular oxygen observed by direct photoproduction from carbon dioxide. Physical Review A, 2017, 95, .	1.0	13
42	Time-resolved measurement of internal conversion dynamics in strong-field molecular ionization. Physical Review A, 2017, 96, .	1.0	9
43	Machine learning molecular dynamics for the simulation of infrared spectra. Chemical Science, 2017, 8, 6924-6935.	3.7	349
44	The DNA nucleobase thymine in motion â€“ Intersystem crossing simulated with surface hopping. Chemical Physics, 2017, 482, 9-15.	0.9	32
45	Challenges in Simulating Light-Induced Processes in DNA. Molecules, 2017, 22, 49.	1.7	21
46	Direct observation of laser-induced O<inf>2</inf>⁺ production from CO<inf>2</inf>. , 2017, , .		0
47	Laser-Induced Oxygen Formation from Carbon Dioxide. Journal of Physics: Conference Series, 2017, 875, 032024.	0.3	0
48	Comparing the accuracy of high-dimensional neural network potentials and the systematic molecular fragmentation method: A benchmark study for all-trans alkanes. Journal of Chemical Physics, 2016, 144, 194110.	1.2	48
49	Communication: GAIMSâ€”Generalized Ab Initio Multiple Spawning for both internal conversion and intersystem crossing processes. Journal of Chemical Physics, 2016, 144, 101102.	1.2	93
50	Photoelectron spectra of 2-thiouracil, 4-thiouracil, and 2,4-dithiouracil. Journal of Chemical Physics, 2016, 144, 074303.	1.2	46
51	Internal conversion and intersystem crossing pathways in UV excited, isolated uracils and their implications in prebiotic chemistry. Physical Chemistry Chemical Physics, 2016, 18, 20168-20176.	1.3	65
52	Intersystem Crossing Pathways in the Noncanonical Nucleobase 2-Thiouracil: A Time-Dependent Picture. Journal of Physical Chemistry Letters, 2016, 7, 1978-1983.	2.1	117
53	Cyclobutane Thymine Photodimerization Mechanism Revealed by Nonadiabatic Molecular Dynamics. Journal of the American Chemical Society, 2016, 138, 15911-15916.	6.6	69
54	Nonadiabatic dynamics and multiphoton resonances in strong-field molecular ionization with few-cycle laser pulses. Physical Review A, 2016, 93, .	1.0	22

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55	The origin of efficient triplet state population in sulfur-substituted nucleobases. Nature Communications, 2016, 7, 13077.	5.8	149
56	Revealing Deactivation Pathways Hidden in Time-Resolved Photoelectron Spectra. Scientific Reports, 2016, 6, 35522.	1.6	27
57	Efficient and Flexible Computation of Many-Electron Wave Function Overlaps. Journal of Chemical Theory and Computation, 2016, 12, 1207-1219.	2.3	145
58	Strong Field Molecular Ionization in the Impulsive Limit: Freezing Vibrations with Short Pulses. Physical Review Letters, 2016, 116, 063002.	2.9	32
59	Additive polarizabilities in ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 1665-1670.	1.3	37
60	A general method to describe intersystem crossing dynamics in trajectory surface hopping. International Journal of Quantum Chemistry, 2015, 115, 1215-1231.	1.0	228
61	A spectroscopic study of the cis/trans-isomers of penta-2,4-dienoic acid attached to gold nanoclusters. Physical Chemistry Chemical Physics, 2015, 17, 7648-7658.	1.3	8
62	High-Dimensional Neural Network Potentials for Organic Reactions and an Improved Training Algorithm. Journal of Chemical Theory and Computation, 2015, 11, 2187-2198.	2.3	105
63	Electronic and Structural Elements That Regulate the Excited-State Dynamics in Purine Nucleobase Derivatives. Journal of the American Chemical Society, 2015, 137, 4368-4381.	6.6	72
64	A Static Picture of the Relaxation and Intersystem Crossing Mechanisms of Photoexcited 2-Thiouracil. Journal of Physical Chemistry A, 2015, 119, 9524-9533.	1.1	69
65	Ultrafast Intersystem Crossing in SO2 and Nucleobases. Springer Proceedings in Physics, 2015, , 509-513.	0.1	1
66	Excitation of Nucleobases from a Computational Perspective II: Dynamics. Topics in Current Chemistry, 2014, 355, 99-153.	4.0	43
67	Non-adiabatic and intersystem crossing dynamics in SO₂. II. The role of triplet states in the bound state dynamics studied by surface-hopping simulations. Journal of Chemical Physics, 2014, 140, 204302.	1.2	68
68	Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. Journal of Chemical Physics, 2014, 141, 074105.	1.2	33
69	Ultrafast intersystem crossing dynamics in uracil unravelled byab initiomolecular dynamics. Physical Chemistry Chemical Physics, 2014, 16, 24423-24436.	1.3	95
70	Chapter 1: Vibrational and Electronic Wavepackets Driven by Strong Field Multiphoton Ionization. Advances in Multi-photon Processes and Spectroscopy, 2014, , 1-54.	0.6	2
71	Ultrafast Laser-Induced Processes Described by Ab Initio Molecular Dynamics. Springer Series in Chemical Physics, 2014, , 145-170.	0.2	4
72	Ultrafast Intersystem Crossing in SO2 and Nucleobases. , 2014, , .		0

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73	Singlet and Triplet Excitedâ€State Dynamics Study of the Keto and Enol Tautomers of Cytosine. ChemPhysChem, 2013, 14, 2920-2931.	1.0	86
74	Distinguishing chemical and electromagnetic enhancement in surfaceâ€enhanced Raman spectra: The case of paraâ€nitrothiophenol. Journal of Raman Spectroscopy, 2013, 44, 1497-1505.	1.2	36
75	Resonance Raman spectra of ortho-nitrophenol calculated by real-time time-dependent density functional theory. Journal of Chemical Physics, 2013, 138, 044101.	1.2	24
76	Control of Nuclear Dynamics with Strong Ultrashort Laser Pulses. Journal of Physical Chemistry A, 2012, 116, 11434-11440.	1.1	33
77	Mixed Quantum-Classical Dynamics in the Adiabatic Representation To Simulate Molecules Driven by Strong Laser Pulses. Journal of Physical Chemistry A, 2012, 116, 2800-2807.	1.1	42
78	Stark Control of a Chiral Fluoroethylene Derivative. Journal of Physical Chemistry A, 2012, 116, 2743-2749.	1.1	15
79	Correction to â€œSHARC â€“ Ab Initio Molecular Dynamics with Surface Hopping in the Adiabatic Representation Including Arbitrary Couplingsâ€•[J. Chem. Theory Comput.2011, 7, 1253â€“1258]. Journal of Chemical Theory and Computation, 2012, 8, 374-374.	2.3	10
80	Femtosecond Intersystem Crossing in the DNA Nucleobase Cytosine. Journal of Physical Chemistry Letters, 2012, 3, 3090-3095.	2.1	146
81	SHARC: ab Initio Molecular Dynamics with Surface Hopping in the Adiabatic Representation Including Arbitrary Couplings. Journal of Chemical Theory and Computation, 2011, 7, 1253-1258.	2.3	424
82	Nonadiabatic ab initio molecular dynamics including spinâ€“orbit coupling and laser fields. Faraday Discussions, 2011, 153, 261.	1.6	59
83	Pulse-shape-dependent strong-field ionization viewed with velocity-map imaging. Physical Review A, 2011, 84, .	1.0	17
84	On the divergence of time-dependent perturbation theory applied to laser-induced molecular transitions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2009, 42, 195402.	0.6	11
85	Molecular dump processes induced by chirped laser pulses. Journal of Chemical Physics, 2008, 129, 074303.	1.2	9
86	Analysis of laser fields for photoassociation and molecular stabilization derived from local control theory. Journal of Physics B: Atomic, Molecular and Optical Physics, 2008, 41, 074026.	0.6	9
87	Local control theory applied to molecular photoassociation. Journal of Chemical Physics, 2007, 127, 084115.	1.2	44
88	Properties of wave packets deduced from quantum control fitness landscapes. Europhysics Letters, 2007, 80, 53001.	0.7	23
89	Photoluminescence and Conductivity of Self-Assembled Ï€â€“Ï€ Stacks of Perylene Bisimide Dyes. Chemistry - A European Journal, 2007, 13, 436-449.	1.7	552
90	On the geometry dependence of molecular dimer spectra with an application to aggregates of perylene bisimide. Chemical Physics, 2006, 328, 354-362.	0.9	165

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91	Complete local control of molecular excited state photo-fragmentation. Chemical Physics Letters, 2006, 426, 263-267.	1.2	10
92	Application of a reflection principle to spectroscopic transitions in molecular dimers. Chemical Physics Letters, 2006, 433, 199-203.	1.2	3
93	Classical aspects emerging from local control of energy and particle transfer in molecules. Journal of Photochemistry and Photobiology A: Chemistry, 2006, 180, 271-276.	2.0	6
94	Local control of the quantum dynamics in multiple potential wells. Journal of Chemical Physics, 2006, 124, 054325.	1.2	23
95	Predissociation and dissociation dynamics in quantum control fields. Chemical Physics Letters, 2005, 407, 471-476.	1.2	19
96	Local control of molecular fragmentation: The role of orientation. Journal of Chemical Physics, 2005, 123, 204320.	1.2	25
97	Femtosecond pulse induced predissociation dynamics in static electric fields. Physical Chemistry Chemical Physics, 2005, 7, 469.	1.3	9
98	Molecular orientation via a dynamically induced pulse-train: Wave packet dynamics of NaI in a static electric field. Journal of Chemical Physics, 2004, 120, 5871-5874.	1.2	27
99	Quantum control fields from instantaneous dynamics. Chemical Physics Letters, 2004, 398, 180-185.	1.2	18
100	Combined electronic and nuclear dynamics in a simple model system. Journal of Chemical Physics, 2003, 119, 672-679.	1.2	30