Philipp Marquetand

List of Publications by Year in Descending Order

98 papers	4,380 citations	32 h-index	65 g-index
106 ext. papers	5,190 ext. citations	5.1 avg, IF	6.2 L-index

#	Paper	IF	Citations
98	BuRNN: Buffer Region Neural Network Approach for Polarizable-Embedding Neural Network/Molecular Mechanics Simulations.. *Journal of Physical Chemistry Letters*, **2022**, 3812-3818	6.4	4
97	Solving the electronic Schrödinger equation for multiple nuclear geometries with weight-sharing deep neural networks. *Nature Computational Science*, **2022**, 2, 331-341		2
96	Machine Learning for Electronically Excited States of Molecules. *Chemical Reviews*, **2021**, 121, 9873-9926	68.1	79
95	A Force Field for a Manganese-Vanadium Water Oxidation Catalyst: Redox Potentials in Solution as Showcase. *Catalysts*, **2021**, 11, 493	4	1
94	Tridentate 3-Substituted Naphthoquinone Ruthenium Arene Complexes: Synthesis, Characterization, Aqueous Behavior, and Theoretical and Biological Studies. *Inorganic Chemistry*, **2021**, 60, 9805-9819	5.1	2
93	Photo-Initiated Cobalt-Catalyzed Radical Olefin Hydrogenation. *Chemistry - A European Journal*, **2021**, 27, 16978-16989	4.8	1
92	Ultrafast photochemistry of a molybdenum carbonyl-nitrosyl complex with a triazacyclononane coligand. *Physical Chemistry Chemical Physics*, **2021**, 23, 24187-24199	3.6	0
91	Competition between dynamic resonance and internal conversion in strong-field molecular ionization with chirped ultrafast laser pulses. *Physical Review A*, **2021**, 103,	2.6	1
90	Activation by oxidation and ligand exchange in a molecular manganese vanadium oxide water oxidation catalyst. *Chemical Science*, **2021**, 12, 12918-12927	9.4	5
89	Excited-state dynamics of CHI and CHIBr studied with UV-pump VUV-probe momentum-resolved photoion spectroscopy. *Journal of Chemical Physics*, **2020**, 153, 184304	3.9	2
88	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	5.1	32
87	Combining SchNet and SHARC: The SchNarc Machine Learning Approach for Excited-State Dynamics. *Journal of Physical Chemistry Letters*, **2020**, 11, 3828-3834	6.4	63
86	Molecular Dynamics with Neural Network Potentials. *Lecture Notes in Physics*, **2020**, 233-252	0.8	6
85	Chapter 4:Machine Learning for Nonadiabatic Molecular Dynamics. *RSC Theoretical and Computational Chemistry Series*, **2020**, 76-108	1.2	2
84	Machine learning and excited-state molecular dynamics. *Machine Learning: Science and Technology*, **2020**, 1, 043001	5.1	30
83	Adiabatic elimination in strong-field light-matter coupling. *Physical Review A*, **2020**, 102,	2.6	1
82	Surface Hopping Molecular Dynamics **2020**, 499-530		4

81	Coherent Control of Internal Conversion in Strong-Field Molecular Ionization. *Physical Review Letters*, **2020**, 125, 053202	7.4	5
80	Deep learning for UV absorption spectra with SchNarc: First steps toward transferability in chemical compound space. *Journal of Chemical Physics*, **2020**, 153, 154112	3.9	21
79	Spectroscopic and Structural Probing of Excited-State Molecular Dynamics with Time-Resolved Photoelectron Spectroscopy and Ultrafast Electron Diffraction. *Physical Review X*, **2020**, 10,	9.1	7
78	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.4	310
77	Excited state dynamics of CHI and CHBrI studied with UV pump VUV probe photoelectron spectroscopy. *Journal of Chemical Physics*, **2019**, 150, 174201	3.9	14
76	Machine learning enables long time scale molecular photodynamics simulations. *Chemical Science*, **2019**, 10, 8100-8107	9.4	96
75	Exploring density functional subspaces with genetic algorithms. *Monatshefte Fü Chemie*, **2019**, 150, 173-182	1.4	6
74	wACSF-Weighted atom-centered symmetry functions as descriptors in machine learning potentials. *Journal of Chemical Physics*, **2018**, 148, 241709	3.9	130
73	Machine Learning for Organic Synthesis: Are Robots Replacing Chemists?. *Angewandte Chemie - International Edition*, **2018**, 57, 6978-6980	16.4	44
72	Nonadiabatic dynamics: The SHARC approach. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1370	7.9	158
71	Maschinelles Lernen fü die organische Synthese: Ersetzen Roboter Chemiker?. *Angewandte Chemie* , **2018**, 130, 7096-7098	3.6	8
70	Stepwise photosensitized thymine dimerization mediated by an exciton intermediate. *Monatshefte Fü Chemie*, **2018**, 149, 1-9	1.4	13
69	Strong-field- versus weak-field-ionization pump-probe spectroscopy. *Physical Review A*, **2018**, 98,	2.6	12
68	Simulated and Experimental Time-Resolved Photoelectron Spectra of the Intersystem Crossing Dynamics in 2-Thiouracil. *Molecules*, **2018**, 23,	4.8	19
67	Cover Image, Volume 8, Issue 6. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1400	7.9	7
66	Ab initio molecular dynamics relaxation and intersystem crossing mechanisms of 5-azacytosine. *Physical Chemistry Chemical Physics*, **2017**, 19, 5888-5894	3.6	24
65	Solvatochromic Effects on the Absorption Spectrum of 2-Thiocytosine. *Journal of Physical Chemistry B*, **2017**, 121, 5187-5196	3.4	19
64	2-Thiouracil intersystem crossing photodynamics studied by wavelength-dependent photoelectron and transient absorption spectroscopies. *Physical Chemistry Chemical Physics*, **2017**, 19, 19756-19766	3.6	43

63	Publisher's Note: Molecular oxygen observed by direct photoproduction from carbon dioxide [Phys. Rev. A 95, 011404(R) (2017)]. *Physical Review A*, **2017**, 95,	2.6	2
62	Ionic dynamics underlying strong-field dissociative molecular ionization. *Physical Review A*, **2017**, 96,	2.6	3
61	Laser-Induced Oxygen Formation from Carbon Dioxide. *Journal of Physics: Conference Series*, **2017**, 875, 032024	0.3	
60	Molecular oxygen observed by direct photoproduction from carbon dioxide. *Physical Review A*, **2017**, 95,	2.6	7
59	Time-resolved measurement of internal conversion dynamics in strong-field molecular ionization. *Physical Review A*, **2017**, 96,	2.6	5
58	Machine learning molecular dynamics for the simulation of infrared spectra. *Chemical Science*, **2017**, 8, 6924-6935	9.4	237
57	The DNA nucleobase thymine in motion – intersystem crossing simulated with surface hopping. *Chemical Physics*, **2017**, 482, 9-15	2.3	27
56	Challenges in Simulating Light-Induced Processes in DNA. *Molecules*, **2017**, 22, 49	4.8	13
55	Nonadiabatic dynamics and multiphoton resonances in strong-field molecular ionization with few-cycle laser pulses. *Physical Review A*, **2016**, 93,	2.6	18
54	The origin of efficient triplet state population in sulfur-substituted nucleobases. *Nature Communications*, **2016**, 7, 13077	17.4	110
53	Revealing Deactivation Pathways Hidden in Time-Resolved Photoelectron Spectra. *Scientific Reports*, **2016**, 6, 35522	4.9	21
52	Efficient and Flexible Computation of Many-Electron Wave Function Overlaps. *Journal of Chemical Theory and Computation*, **2016**, 12, 1207-19	6.4	100
51	Strong Field Molecular Ionization in the Impulsive Limit: Freezing Vibrations with Short Pulses. *Physical Review Letters*, **2016**, 116, 063002	7.4	25
50	Additive polarizabilities in ionic liquids. *Physical Chemistry Chemical Physics*, **2016**, 18, 1665-70	3.6	27
49	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	3.9	39
48	Communication: GAIMS--Generalized Ab Initio Multiple Spawning for both internal conversion and intersystem crossing processes. *Journal of Chemical Physics*, **2016**, 144, 101102	3.9	74
47	Photoelectron spectra of 2-thiouracil, 4-thiouracil, and 2,4-dithiouracil. *Journal of Chemical Physics*, **2016**, 144, 074303	3.9	37
46	Internal conversion and intersystem crossing pathways in UV excited, isolated uracils and their implications in prebiotic chemistry. *Physical Chemistry Chemical Physics*, **2016**, 18, 20168-76	3.6	50

45	Intersystem Crossing Pathways in the Noncanonical Nucleobase 2-Thiouracil: A Time-Dependent Picture. *Journal of Physical Chemistry Letters*, **2016**, 7, 1978-83	6.4	97
44	Cyclobutane Thymine Photodimerization Mechanism Revealed by Nonadiabatic Molecular Dynamics. *Journal of the American Chemical Society*, **2016**, 138, 15911-15916	16.4	48
43	High-Dimensional Neural Network Potentials for Organic Reactions and an Improved Training Algorithm. *Journal of Chemical Theory and Computation*, **2015**, 11, 2187-98	6.4	87
42	Electronic and structural elements that regulate the excited-state dynamics in purine nucleobase derivatives. *Journal of the American Chemical Society*, **2015**, 137, 4368-81	16.4	58
41	A Static Picture of the Relaxation and Intersystem Crossing Mechanisms of Photoexcited 2-Thiouracil. *Journal of Physical Chemistry A*, **2015**, 119, 9524-33	2.8	55
40	A general method to describe intersystem crossing dynamics in trajectory surface hopping. *International Journal of Quantum Chemistry*, **2015**, 115, 1215-1231	2.1	178
39	A spectroscopic study of the cis/trans-isomers of penta-2,4-dienoic acid attached to gold nanoclusters. *Physical Chemistry Chemical Physics*, **2015**, 17, 7648-58	3.6	7
38	Excitation of nucleobases from a computational perspective II: dynamics. *Topics in Current Chemistry*, **2015**, 355, 99-153		37
37	Ultrafast Intersystem Crossing in SO2 and Nucleobases. *Springer Proceedings in Physics*, **2015**, 509-513	0.2	1
36	Ultrafast intersystem crossing dynamics in uracil unravelled by ab initio molecular dynamics. *Physical Chemistry Chemical Physics*, **2014**, 16, 24423-36	3.6	80
35	Chapter 1: Vibrational and Electronic Wavepackets Driven by Strong Field Multiphoton Ionization. *Advances in Multi-photon Processes and Spectroscopy*, **2014**, 1-54		2
34	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	3.9	58
33	Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. *Journal of Chemical Physics*, **2014**, 141, 074105	3.9	24
32	Ultrafast Laser-Induced Processes Described by Ab Initio Molecular Dynamics. *Springer Series in Chemical Physics*, **2014**, 145-170	0.3	3
31	Singlet and triplet excited-state dynamics study of the keto and enol tautomers of cytosine. *ChemPhysChem*, **2013**, 14, 2920-31	3.2	75
30	Distinguishing chemical and electromagnetic enhancement in surface-enhanced Raman spectra: The case of para-nitrothiophenol. *Journal of Raman Spectroscopy*, **2013**, 44, 1497-1505	2.3	28
29	Resonance Raman spectra of ortho-nitrophenol calculated by real-time time-dependent density functional theory. *Journal of Chemical Physics*, **2013**, 138, 044101	3.9	21
28	Control of nuclear dynamics with strong ultrashort laser pulses. *Journal of Physical Chemistry A*, **2012**, 116, 11434-40	2.8	27

27	Mixed quantum-classical dynamics in the adiabatic representation to simulate molecules driven by strong laser pulses. *Journal of Physical Chemistry A*, **2012**, 116, 2800-7	2.8	37
26	Stark control of a chiral fluoroethylene derivative. *Journal of Physical Chemistry A*, **2012**, 116, 2743-9	2.8	15
25	Correction to "SHARC - Ab Initio Molecular Dynamics with Surface Hopping in the Adiabatic Representation Including Arbitrary Couplings" [J. Chem. Theory Comput.2011, 7, 1253-1258]. *Journal of Chemical Theory and Computation*, **2012**, 8, 374	6.4	6
24	Femtosecond Intersystem Crossing in the DNA Nucleobase Cytosine. *Journal of Physical Chemistry Letters*, **2012**, 3, 3090-5	6.4	134
23	Nonadiabatic ab initio molecular dynamics including spin-orbit coupling and laser fields. *Faraday Discussions*, **2011**, 153, 261-73; discussion 293-319	3.6	54
22	SHARC: ab Initio Molecular Dynamics with Surface Hopping in the Adiabatic Representation Including Arbitrary Couplings. *Journal of Chemical Theory and Computation*, **2011**, 7, 1253-8	6.4	329
21	Pulse-shape-dependent strong-field ionization viewed with velocity-map imaging. *Physical Review A* , **2011**, 84,	2.6	17
20	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	1.3	10
19	Molecular dump processes induced by chirped laser pulses. *Journal of Chemical Physics*, **2008**, 129, 074303	3.9	8
18	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	1.3	9
17	Photoluminescence and conductivity of self-assembled pi-pi stacks of perylene bisimide dyes. *Chemistry - A European Journal*, **2007**, 13, 436-49	4.8	517
16	Local control theory applied to molecular photoassociation. *Journal of Chemical Physics*, **2007**, 127, 084115	3.9	42
15	Properties of wave packets deduced from quantum control fitness landscapes. *Europhysics Letters*, **2007**, 80, 53001	1.6	22
14	Local control of the quantum dynamics in multiple potential wells. *Journal of Chemical Physics*, **2006** , 124, 054325	3.9	23
13	On the geometry dependence of molecular dimer spectra with an application to aggregates of perylene bisimide. *Chemical Physics*, **2006**, 328, 354-362	2.3	157
12	Complete local control of molecular excited state photo-fragmentation. *Chemical Physics Letters*, **2006**, 426, 263-267	2.5	10
11	Application of a reflection principle to spectroscopic transitions in molecular dimers. *Chemical Physics Letters*, **2006**, 433, 199-203	2.5	3
10	Classical aspects emerging from local control of energy and particle transfer in molecules. *Journal of Photochemistry and Photobiology A: Chemistry*, **2006**, 180, 271-276	4.7	6

9	Femtosecond pulse induced predissociation dynamics in static electric fields. *Physical Chemistry Chemical Physics*, **2005**, 7, 469	3.6	9
8	Predissociation and dissociation dynamics in quantum control fields. *Chemical Physics Letters*, **2005**, 407, 471-476	2.5	19
7	Local control of molecular fragmentation: the role of orientation. *Journal of Chemical Physics*, **2005**, 123, 204320	3.9	22
6	Molecular orientation via a dynamically induced pulse-train: wave packet dynamics of NaI in a static electric field. *Journal of Chemical Physics*, **2004**, 120, 5871-4	3.9	26
5	Quantum control fields from instantaneous dynamics. *Chemical Physics Letters*, **2004**, 398, 180-185	2.5	18
4	Combined electronic and nuclear dynamics in a simple model system. *Journal of Chemical Physics*, **2003**, 119, 672-679	3.9	27
3	OpenMolcas: From Source Code to Insight		4
2	CHAPTER 10:General Trajectory Surface Hopping Method for Ultrafast Nonadiabatic Dynamics. *RSC Theoretical and Computational Chemistry Series*,348-385	1.2	1
1	Deep learning study of tyrosine reveals that roaming can lead to photodamage. *Nature Chemistry*,	17.6	3