

# Philipp Marquetand

## List of Publications by Year in descending order

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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	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5925-5964.	2.3	661
2	Photoluminescence and Conductivity of Self-Assembled $\pi$ - $\pi$ Stacks of Perylene Bisimide Dyes. <i>Chemistry - A European Journal</i> , 2007, 13, 436-449.	1.7	552
3	SHARC: <i>ab Initio</i> Molecular Dynamics with Surface Hopping in the Adiabatic Representation Including Arbitrary Couplings. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1253-1258.	2.3	424
4	Machine learning molecular dynamics for the simulation of infrared spectra. <i>Chemical Science</i> , 2017, 8, 6924-6935.	3.7	349
5	Nonadiabatic dynamics: The SHARC approach. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018, 8, e1370.	6.2	274
6	A general method to describe intersystem crossing dynamics in trajectory surface hopping. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1215-1231.	1.0	228
7	Machine Learning for Electronically Excited States of Molecules. <i>Chemical Reviews</i> , 2021, 121, 9873-9926.	23.0	207
8	wACSF $\pi$ Weighted atom-centered symmetry functions as descriptors in machine learning potentials. <i>Journal of Chemical Physics</i> , 2018, 148, 241709.	1.2	198
9	On the geometry dependence of molecular dimer spectra with an application to aggregates of perylene bisimide. <i>Chemical Physics</i> , 2006, 328, 354-362.	0.9	165
10	The origin of efficient triplet state population in sulfur-substituted nucleobases. <i>Nature Communications</i> , 2016, 7, 13077.	5.8	149
11	Femtosecond Intersystem Crossing in the DNA Nucleobase Cytosine. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3090-3095.	2.1	146
12	Efficient and Flexible Computation of Many-Electron Wave Function Overlaps. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1207-1219.	2.3	145
13	Machine learning enables long time scale molecular photodynamics simulations. <i>Chemical Science</i> , 2019, 10, 8100-8107.	3.7	140
14	Intersystem Crossing Pathways in the Noncanonical Nucleobase 2-Thiouracil: A Time-Dependent Picture. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1978-1983.	2.1	117
15	Combining SchNet and SHARC: The SchNarc Machine Learning Approach for Excited-State Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3828-3834.	2.1	114
16	High-Dimensional Neural Network Potentials for Organic Reactions and an Improved Training Algorithm. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2187-2198.	2.3	105
17	Ultrafast intersystem crossing dynamics in uracil unravelled by <i>ab initio</i> molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24423-24436.	1.3	95
18	Communication: GAIMS $\pi$ Generalized <i>Ab Initio</i> Multiple Spawning for both internal conversion and intersystem crossing processes. <i>Journal of Chemical Physics</i> , 2016, 144, 101102.	1.2	93

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19	Singlet and Triplet Excited-State Dynamics Study of the Keto and Enol Tautomers of Cytosine. <i>ChemPhysChem</i> , 2013, 14, 2920-2931.	1.0	86
20	Electronic and Structural Elements That Regulate the Excited-State Dynamics in Purine Nucleobase Derivatives. <i>Journal of the American Chemical Society</i> , 2015, 137, 4368-4381.	6.6	72
21	A Static Picture of the Relaxation and Intersystem Crossing Mechanisms of Photoexcited 2-Thiouracil. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9524-9533.	1.1	69
22	Cyclobutane Thymine Photodimerization Mechanism Revealed by Nonadiabatic Molecular Dynamics. <i>Journal of the American Chemical Society</i> , 2016, 138, 15911-15916.	6.6	69
23	Non-adiabatic and intersystem crossing dynamics in $SO_2$ . II. The role of triplet states in the bound state dynamics studied by surface-hopping simulations. <i>Journal of Chemical Physics</i> , 2014, 140, 204302.	1.2	68
24	Internal conversion and intersystem crossing pathways in UV excited, isolated uracils and their implications in prebiotic chemistry. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20168-20176.	1.3	65
25	Nonadiabatic ab initio molecular dynamics including spin-orbit coupling and laser fields. <i>Faraday Discussions</i> , 2011, 153, 261.	1.6	59
26	2-Thiouracil intersystem crossing photodynamics studied by wavelength-dependent photoelectron and transient absorption spectroscopies. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 19756-19766.	1.3	58
27	Machine Learning for Organic Synthesis: Are Robots Replacing Chemists?. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 6978-6980.	7.2	56
28	Deep learning for UV absorption spectra with SchNarc: First steps toward transferability in chemical compound space. <i>Journal of Chemical Physics</i> , 2020, 153, 154112.	1.2	50
29	Machine learning and excited-state molecular dynamics. <i>Machine Learning: Science and Technology</i> , 2020, 1, 043001.	2.4	50
30	Comparing the accuracy of high-dimensional neural network potentials and the systematic molecular fragmentation method: A benchmark study for all-trans alkanes. <i>Journal of Chemical Physics</i> , 2016, 144, 194110.	1.2	48
31	Neural networks and kernel ridge regression for excited states dynamics of $CH_2NH_2^+$ : From single-state to multi-state representations and multi-property machine learning models. <i>Machine Learning: Science and Technology</i> , 2020, 1, 025009.	2.4	47
32	Photoelectron spectra of 2-thiouracil, 4-thiouracil, and 2,4-dithiouracil. <i>Journal of Chemical Physics</i> , 2016, 144, 074303.	1.2	46
33	Local control theory applied to molecular photoassociation. <i>Journal of Chemical Physics</i> , 2007, 127, 084115.	1.2	44
34	Excitation of Nucleobases from a Computational Perspective II: Dynamics. <i>Topics in Current Chemistry</i> , 2014, 355, 99-153.	4.0	43
35	Mixed Quantum-Classical Dynamics in the Adiabatic Representation To Simulate Molecules Driven by Strong Laser Pulses. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2800-2807.	1.1	42
36	Additive polarizabilities in ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1665-1670.	1.3	37

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37	Distinguishing chemical and electromagnetic enhancement in surface-enhanced Raman spectra: The case of <i>para</i> -nitrothiophenol. Journal of Raman Spectroscopy, 2013, 44, 1497-1505.	1.2	36
38	Control of Nuclear Dynamics with Strong Ultrashort Laser Pulses. Journal of Physical Chemistry A, 2012, 116, 11434-11440.	1.1	33
39	Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. Journal of Chemical Physics, 2014, 141, 074105.	1.2	33
40	Strong Field Molecular Ionization in the Impulsive Limit: Freezing Vibrations with Short Pulses. Physical Review Letters, 2016, 116, 063002.	2.9	32
41	The DNA nucleobase thymine in motion – Intersystem crossing simulated with surface hopping. Chemical Physics, 2017, 482, 9-15.	0.9	32
42	Ab initio molecular dynamics relaxation and intersystem crossing mechanisms of 5-azacytosine. Physical Chemistry Chemical Physics, 2017, 19, 5888-5894.	1.3	31
43	Solvatochromic Effects on the Absorption Spectrum of 2-Thiocytosine. Journal of Physical Chemistry B, 2017, 121, 5187-5196.	1.2	31
44	Combined electronic and nuclear dynamics in a simple model system. Journal of Chemical Physics, 2003, 119, 672-679.	1.2	30
45	Simulated and Experimental Time-Resolved Photoelectron Spectra of the Intersystem Crossing Dynamics in 2-Thiouracil. Molecules, 2018, 23, 2836.	1.7	28
46	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
47	Revealing Deactivation Pathways Hidden in Time-Resolved Photoelectron Spectra. Scientific Reports, 2016, 6, 35522.	1.6	27
48	Local control of molecular fragmentation: The role of orientation. Journal of Chemical Physics, 2005, 123, 204320.	1.2	25
49	Solving the electronic Schrödinger equation for multiple nuclear geometries with weight-sharing deep neural networks. Nature Computational Science, 2022, 2, 331-341.	3.8	25
50	Resonance Raman spectra of <i>ortho</i> -nitrophenol calculated by real-time time-dependent density functional theory. Journal of Chemical Physics, 2013, 138, 044101.	1.2	24
51	Local control of the quantum dynamics in multiple potential wells. Journal of Chemical Physics, 2006, 124, 054325.	1.2	23
52	Properties of wave packets deduced from quantum control fitness landscapes. Europhysics Letters, 2007, 80, 53001.	0.7	23
53	Excited state dynamics of CH <sub>2</sub> I <sub>2</sub> and CH <sub>2</sub> BrI studied with UV pump VUV probe photoelectron spectroscopy. Journal of Chemical Physics, 2019, 150, 174201.	1.2	23
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	Challenges in Simulating Light-Induced Processes in DNA. <i>Molecules</i> , 2017, 22, 49.	1.7	21
56	Deep learning study of tyrosine reveals that roaming can lead to photodamage. <i>Nature Chemistry</i> , 2022, 14, 914-919.	6.6	21
57	Predissociation and dissociation dynamics in quantum control fields. <i>Chemical Physics Letters</i> , 2005, 407, 471-476.	1.2	19
58	Quantum control fields from instantaneous dynamics. <i>Chemical Physics Letters</i> , 2004, 398, 180-185.	1.2	18
59	BuRNN: Buffer Region Neural Network Approach for Polarizable-Embedding Neural Network/Molecular Mechanics Simulations. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3812-3818.	2.1	18
60	Pulse-shape-dependent strong-field ionization viewed with velocity-map imaging. <i>Physical Review A</i> , 2011, 84, .	1.0	17
61	Strong-field- versus weak-field-ionization pump-probe spectroscopy. <i>Physical Review A</i> , 2018, 98, .	1.0	16
62	Stark Control of a Chiral Fluoroethylene Derivative. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2743-2749.	1.1	15
63	Stepwise photosensitized thymine dimerization mediated by an exciton intermediate. <i>Monatshefte für Chemie</i> , 2018, 149, 1-9.	0.9	14
64	Molecular oxygen observed by direct photoproduction from carbon dioxide. <i>Physical Review A</i> , 2017, 95, .	1.0	13
65	Molecular Dynamics with Neural Network Potentials. <i>Lecture Notes in Physics</i> , 2020, , 233-252.	0.3	12
66	On the divergence of time-dependent perturbation theory applied to laser-induced molecular transitions. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2009, 42, 195402.	0.6	11
67	Spectroscopic and Structural Probing of Excited-State Molecular Dynamics with Time-Resolved Photoelectron Spectroscopy and Ultrafast Electron Diffraction. <i>Physical Review X</i> , 2020, 10, .	2.8	11
68	Adiabatic elimination in strong-field light-matter coupling. <i>Physical Review A</i> , 2020, 102, .	1.0	11
69	Complete local control of molecular excited state photo-fragmentation. <i>Chemical Physics Letters</i> , 2006, 426, 263-267.	1.2	10
70	Correction to "SHARC: Ab Initio Molecular Dynamics with Surface Hopping in the Adiabatic Representation Including Arbitrary Couplings". <i>Chem. Theory Comput.</i> 2011, 7, 1253-1258. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 374-374.	2.3	10
71	Coherent Control of Internal Conversion in Strong-Field Molecular Ionization. <i>Physical Review Letters</i> , 2020, 125, 053202.	2.9	10
72	Activation by oxidation and ligand exchange in a molecular manganese vanadium oxide water oxidation catalyst. <i>Chemical Science</i> , 2021, 12, 12918-12927.	3.7	10

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73	Femtosecond pulse induced predissociation dynamics in static electric fields. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 469.	1.3	9
74	Molecular dump processes induced by chirped laser pulses. <i>Journal of Chemical Physics</i> , 2008, 129, 074303.	1.2	9
75	Analysis of laser fields for photoassociation and molecular stabilization derived from local control theory. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2008, 41, 074026.	0.6	9
76	Time-resolved measurement of internal conversion dynamics in strong-field molecular ionization. <i>Physical Review A</i> , 2017, 96, .	1.0	9
77	Excited-state dynamics of CH <sub>2</sub> I <sub>2</sub> and CH <sub>2</sub> IBr studied with UV-pump VUV-probe momentum-resolved photoion spectroscopy. <i>Journal of Chemical Physics</i> , 2020, 153, 184304.	1.2	9
78	Tridentate 3-Substituted Naphthoquinone Ruthenium Arene Complexes: Synthesis, Characterization, Aqueous Behavior, and Theoretical and Biological Studies. <i>Inorganic Chemistry</i> , 2021, 60, 9805-9819.	1.9	9
79	A spectroscopic study of the cis/trans-isomers of penta-2,4-dienoic acid attached to gold nanoclusters. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7648-7658.	1.3	8
80	Maschinelles Lernen für die organische Synthese: Ersetzen Roboter Chemiker?. <i>Angewandte Chemie</i> , 2018, 130, 7096-7098.	1.6	8
81	Exploring density functional subspaces with genetic algorithms. <i>Monatshefte für Chemie</i> , 2019, 150, 173-182.	0.9	8
82	Competition between dynamic resonance and internal conversion in strong-field molecular ionization with chirped ultrafast laser pulses. <i>Physical Review A</i> , 2021, 103, .	1.0	8
83	A Force Field for a Manganese-Vanadium Water Oxidation Catalyst: Redox Potentials in Solution as Showcase. <i>Catalysts</i> , 2021, 11, 493.	1.6	8
84	Photo-initiated Cobalt-catalyzed Radical Olefin Hydrogenation. <i>Chemistry - A European Journal</i> , 2021, 27, 16978-16989.	1.7	8
85	Cover Image, Volume 8, Issue 6. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018, 8, e1400.	6.2	7
86	Classical aspects emerging from local control of energy and particle transfer in molecules. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2006, 180, 271-276.	2.0	6
87	Ultrafast Laser-Induced Processes Described by Ab Initio Molecular Dynamics. <i>Springer Series in Chemical Physics</i> , 2014, , 145-170.	0.2	4
88	Application of a reflection principle to spectroscopic transitions in molecular dimers. <i>Chemical Physics Letters</i> , 2006, 433, 199-203.	1.2	3
89	Ionic dynamics underlying strong-field dissociative molecular ionization. <i>Physical Review A</i> , 2017, 96, .	1.0	3
90	General Trajectory Surface Hopping Method for Ultrafast Nonadiabatic Dynamics. <i>RSC Theoretical and Computational Chemistry Series</i> , 2018, , 348-385.	0.7	3

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91	Machine Learning for Nonadiabatic Molecular Dynamics. RSC Theoretical and Computational Chemistry Series, 2020, , 76-108.	0.7	3
92	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
93	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
94	Ultrafast photochemistry of a molybdenum carbonylâ€“nitrosyl complex with a triazacyclononane coligand. Physical Chemistry Chemical Physics, 2021, 23, 24187-24199.	1.3	2
95	Ultrafast Intersystem Crossing in SO2 and Nucleobases. Springer Proceedings in Physics, 2015, , 509-513.	0.1	1
96	Direct observation of laser-induced O<sub>2</sub> production from CO<sub>2</sub>. , 2017, , .		0
97	Laser-Induced Oxygen Formation from Carbon Dioxide. Journal of Physics: Conference Series, 2017, 875, 032024.	0.3	0
98	Development of a Hybrid Neural Network/Molecular Mechanics Approach for Metalloprotein Simulations. Biophysical Journal, 2021, 120, 195a.	0.2	0
99	Femtosecond molecular dynamics viewed by multi-model imaging. , 2021, , .		0
100	Ultrafast Intersystem Crossing in SO2 and Nucleobases. , 2014, , .		0