

# Philipp Marquetand

## List of Publications by Citations

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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	Photoluminescence and conductivity of self-assembled pi-pi stacks of perylene bisimide dyes. <i>Chemistry - A European Journal</i> , <b>2007</b> , 13, 436-49	4.8	517
97	SHARC: ab Initio Molecular Dynamics with Surface Hopping in the Adiabatic Representation Including Arbitrary Couplings. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 1253-8	6.4	329
96	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 5925-5964	6.4	310
95	Machine learning molecular dynamics for the simulation of infrared spectra. <i>Chemical Science</i> , <b>2017</b> , 8, 6924-6935	9.4	237
94	A general method to describe intersystem crossing dynamics in trajectory surface hopping. <i>International Journal of Quantum Chemistry</i> , <b>2015</b> , 115, 1215-1231	2.1	178
93	Nonadiabatic dynamics: The SHARC approach. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2018</b> , 8, e1370	7.9	158
92	On the geometry dependence of molecular dimer spectra with an application to aggregates of perylene bisimide. <i>Chemical Physics</i> , <b>2006</b> , 328, 354-362	2.3	157
91	Femtosecond Intersystem Crossing in the DNA Nucleobase Cytosine. <i>Journal of Physical Chemistry Letters</i> , <b>2012</b> , 3, 3090-5	6.4	134
90	wACSF-Weighted atom-centered symmetry functions as descriptors in machine learning potentials. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 241709	3.9	130
89	The origin of efficient triplet state population in sulfur-substituted nucleobases. <i>Nature Communications</i> , <b>2016</b> , 7, 13077	17.4	110
88	Efficient and Flexible Computation of Many-Electron Wave Function Overlaps. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 1207-19	6.4	100
87	Intersystem Crossing Pathways in the Noncanonical Nucleobase 2-Thiouracil: A Time-Dependent Picture. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 1978-83	6.4	97
86	Machine learning enables long time scale molecular photodynamics simulations. <i>Chemical Science</i> , <b>2019</b> , 10, 8100-8107	9.4	96
85	High-Dimensional Neural Network Potentials for Organic Reactions and an Improved Training Algorithm. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 2187-98	6.4	87
84	Ultrafast intersystem crossing dynamics in uracil unravelled by ab initio molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 24423-36	3.6	80
83	Machine Learning for Electronically Excited States of Molecules. <i>Chemical Reviews</i> , <b>2021</b> , 121, 9873-9926	68.1	79
82	Singlet and triplet excited-state dynamics study of the keto and enol tautomers of cytosine. <i>ChemPhysChem</i> , <b>2013</b> , 14, 2920-31	3.2	75

81	Communication: GAIMS--Generalized Ab Initio Multiple Spawning for both internal conversion and intersystem crossing processes. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 101102	3.9	74
80	Combining SchNet and SHARC: The SchNarc Machine Learning Approach for Excited-State Dynamics. <i>Journal of Physical Chemistry Letters</i> , <b>2020</b> , 11, 3828-3834	6.4	63
79	Electronic and structural elements that regulate the excited-state dynamics in purine nucleobase derivatives. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 4368-81	16.4	58
78	Non-adiabatic and intersystem crossing dynamics in SO <sub>2</sub> . II. The role of triplet states in the bound state dynamics studied by surface-hopping simulations. <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 204302	3.9	58
77	A Static Picture of the Relaxation and Intersystem Crossing Mechanisms of Photoexcited 2-Thiouracil. <i>Journal of Physical Chemistry A</i> , <b>2015</b> , 119, 9524-33	2.8	55
76	Nonadiabatic ab initio molecular dynamics including spin-orbit coupling and laser fields. <i>Faraday Discussions</i> , <b>2011</b> , 153, 261-73; discussion 293-319	3.6	54
75	Internal conversion and intersystem crossing pathways in UV excited, isolated uracils and their implications in prebiotic chemistry. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 20168-76	3.6	50
74	Cyclobutane Thymine Photodimerization Mechanism Revealed by Nonadiabatic Molecular Dynamics. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 15911-15916	16.4	48
73	Machine Learning for Organic Synthesis: Are Robots Replacing Chemists?. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 6978-6980	16.4	44
72	2-Thiouracil intersystem crossing photodynamics studied by wavelength-dependent photoelectron and transient absorption spectroscopies. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 19756-19766	3.6	43
71	Local control theory applied to molecular photoassociation. <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 084135	16.4	42
70	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> , <b>2016</b> , 144, 194110	3.9	39
69	Excitation of nucleobases from a computational perspective II: dynamics. <i>Topics in Current Chemistry</i> , <b>2015</b> , 355, 99-153		37
68	Mixed quantum-classical dynamics in the adiabatic representation to simulate molecules driven by strong laser pulses. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 2800-7	2.8	37
67	Photoelectron spectra of 2-thiouracil, 4-thiouracil, and 2,4-dithiouracil. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 074303	3.9	37
66	Neural networks and kernel ridge regression for excited states dynamics of CH <sub>2</sub> NH <sub>2</sub> <sup>+</sup> : From single-state to multi-state representations and multi-property machine learning models. <i>Machine Learning: Science and Technology</i> , <b>2020</b> , 1, 025009	5.1	32
65	Machine learning and excited-state molecular dynamics. <i>Machine Learning: Science and Technology</i> , <b>2020</b> , 1, 043001	5.1	30
64	Distinguishing chemical and electromagnetic enhancement in surface-enhanced Raman spectra: The case of para-nitrothiophenol. <i>Journal of Raman Spectroscopy</i> , <b>2013</b> , 44, 1497-1505	2.3	28

63	Additive polarizabilities in ionic liquids. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 1665-70	3.6	27
62	The DNA nucleobase thymine in motion $\Pi$ ntersystem crossing simulated with surface hopping. <i>Chemical Physics</i> , <b>2017</b> , 482, 9-15	2.3	27
61	Control of nuclear dynamics with strong ultrashort laser pulses. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 11434-40	2.8	27
60	Combined electronic and nuclear dynamics in a simple model system. <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 672-679	3.9	27
59	Molecular orientation via a dynamically induced pulse-train: wave packet dynamics of NaI in a static electric field. <i>Journal of Chemical Physics</i> , <b>2004</b> , 120, 5871-4	3.9	26
58	Strong Field Molecular Ionization in the Impulsive Limit: Freezing Vibrations with Short Pulses. <i>Physical Review Letters</i> , <b>2016</b> , 116, 063002	7.4	25
57	Ab initio molecular dynamics relaxation and intersystem crossing mechanisms of 5-azacytosine. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 5888-5894	3.6	24
56	Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. <i>Journal of Chemical Physics</i> , <b>2014</b> , 141, 074105	3.9	24
55	Local control of the quantum dynamics in multiple potential wells. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 054325	3.9	23
54	Properties of wave packets deduced from quantum control fitness landscapes. <i>Europhysics Letters</i> , <b>2007</b> , 80, 53001	1.6	22
53	Local control of molecular fragmentation: the role of orientation. <i>Journal of Chemical Physics</i> , <b>2005</b> , 123, 204320	3.9	22
52	Revealing Deactivation Pathways Hidden in Time-Resolved Photoelectron Spectra. <i>Scientific Reports</i> , <b>2016</b> , 6, 35522	4.9	21
51	Resonance Raman spectra of ortho-nitrophenol calculated by real-time time-dependent density functional theory. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 044101	3.9	21
50	Deep learning for UV absorption spectra with SchNarc: First steps toward transferability in chemical compound space. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 154112	3.9	21
49	Solvatochromic Effects on the Absorption Spectrum of 2-Thiocytosine. <i>Journal of Physical Chemistry B</i> , <b>2017</b> , 121, 5187-5196	3.4	19
48	Predissociation and dissociation dynamics in quantum control fields. <i>Chemical Physics Letters</i> , <b>2005</b> , 407, 471-476	2.5	19
47	Simulated and Experimental Time-Resolved Photoelectron Spectra of the Intersystem Crossing Dynamics in 2-Thiouracil. <i>Molecules</i> , <b>2018</b> , 23,	4.8	19
46	Nonadiabatic dynamics and multiphoton resonances in strong-field molecular ionization with few-cycle laser pulses. <i>Physical Review A</i> , <b>2016</b> , 93,	2.6	18

45	Quantum control fields from instantaneous dynamics. <i>Chemical Physics Letters</i> , <b>2004</b> , 398, 180-185	2.5	18
44	Pulse-shape-dependent strong-field ionization viewed with velocity-map imaging. <i>Physical Review A</i> , <b>2011</b> , 84,	2.6	17
43	Stark control of a chiral fluoroethylene derivative. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 2743-9	2.8	15
42	Excited state dynamics of CHI and CHBr studied with UV pump VUV probe photoelectron spectroscopy. <i>Journal of Chemical Physics</i> , <b>2019</b> , 150, 174201	3.9	14
41	Challenges in Simulating Light-Induced Processes in DNA. <i>Molecules</i> , <b>2017</b> , 22, 49	4.8	13
40	Stepwise photosensitized thymine dimerization mediated by an exciton intermediate. <i>Monatshefte für Chemie</i> , <b>2018</b> , 149, 1-9	1.4	13
39	Strong-field- versus weak-field-ionization pump-probe spectroscopy. <i>Physical Review A</i> , <b>2018</b> , 98,	2.6	12
38	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> , <b>2009</b> , 42, 195402	1.3	10
37	Complete local control of molecular excited state photo-fragmentation. <i>Chemical Physics Letters</i> , <b>2006</b> , 426, 263-267	2.5	10
36	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> , <b>2008</b> , 41, 074026	1.3	9
35	Femtosecond pulse induced predissociation dynamics in static electric fields. <i>Physical Chemistry Chemical Physics</i> , <b>2005</b> , 7, 469	3.6	9
34	Maschinelles Lernen für die organische Synthese: Ersetzen Roboter Chemiker?. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 7096-7098	3.6	8
33	Molecular dump processes induced by chirped laser pulses. <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 074303	3.9	8
32	Molecular oxygen observed by direct photoproduction from carbon dioxide. <i>Physical Review A</i> , <b>2017</b> , 95,	2.6	7
31	A spectroscopic study of the cis/trans-isomers of penta-2,4-dienoic acid attached to gold nanoclusters. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 7648-58	3.6	7
30	Spectroscopic and Structural Probing of Excited-State Molecular Dynamics with Time-Resolved Photoelectron Spectroscopy and Ultrafast Electron Diffraction. <i>Physical Review X</i> , <b>2020</b> , 10,	9.1	7
29	Cover Image, Volume 8, Issue 6. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2018</b> , 8, e1400	7.9	7
28	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]. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 374	6.4	6

27	Classical aspects emerging from local control of energy and particle transfer in molecules. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , <b>2006</b> , 180, 271-276	4.7	6
26	Molecular Dynamics with Neural Network Potentials. <i>Lecture Notes in Physics</i> , <b>2020</b> , 233-252	0.8	6
25	Exploring density functional subspaces with genetic algorithms. <i>Monatshefte für Chemie</i> , <b>2019</b> , 150, 173-182	1.4	6
24	Time-resolved measurement of internal conversion dynamics in strong-field molecular ionization. <i>Physical Review A</i> , <b>2017</b> , 96,	2.6	5
23	Coherent Control of Internal Conversion in Strong-Field Molecular Ionization. <i>Physical Review Letters</i> , <b>2020</b> , 125, 053202	7.4	5
22	Activation by oxidation and ligand exchange in a molecular manganese vanadium oxide water oxidation catalyst. <i>Chemical Science</i> , <b>2021</b> , 12, 12918-12927	9.4	5
21	OpenMolcas: From Source Code to Insight		4
20	Surface Hopping Molecular Dynamics <b>2020</b> , 499-530		4
19	BuRNN: Buffer Region Neural Network Approach for Polarizable-Embedding Neural Network/Molecular Mechanics Simulations.. <i>Journal of Physical Chemistry Letters</i> , <b>2022</b> , 3812-3818	6.4	4
18	Ionic dynamics underlying strong-field dissociative molecular ionization. <i>Physical Review A</i> , <b>2017</b> , 96,	2.6	3
17	Application of a reflection principle to spectroscopic transitions in molecular dimers. <i>Chemical Physics Letters</i> , <b>2006</b> , 433, 199-203	2.5	3
16	Ultrafast Laser-Induced Processes Described by Ab Initio Molecular Dynamics. <i>Springer Series in Chemical Physics</i> , <b>2014</b> , 145-170	0.3	3
15	Deep learning study of tyrosine reveals that roaming can lead to photodamage. <i>Nature Chemistry</i> ,	17.6	3
14	Publisher's Note: Molecular oxygen observed by direct photoproduction from carbon dioxide [Phys. Rev. A 95, 011404(R) (2017)]. <i>Physical Review A</i> , <b>2017</b> , 95,	2.6	2
13	Excited-state dynamics of CHI and CHIBr studied with UV-pump VUV-probe momentum-resolved photoion spectroscopy. <i>Journal of Chemical Physics</i> , <b>2020</b> , 153, 184304	3.9	2
12	Chapter 1: Vibrational and Electronic Wavepackets Driven by Strong Field Multiphoton Ionization. <i>Advances in Multi-photon Processes and Spectroscopy</i> , <b>2014</b> , 1-54		2
11	Chapter 4: Machine Learning for Nonadiabatic Molecular Dynamics. <i>RSC Theoretical and Computational Chemistry Series</i> , <b>2020</b> , 76-108	1.2	2
10	Tridentate 3-Substituted Naphthoquinone Ruthenium Arene Complexes: Synthesis, Characterization, Aqueous Behavior, and Theoretical and Biological Studies. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 9805-9819	5.1	2

9	Solving the electronic Schrödinger equation for multiple nuclear geometries with weight-sharing deep neural networks. <i>Nature Computational Science</i> , <b>2022</b> , 2, 331-341		2
8	Ultrafast Intersystem Crossing in SO <sub>2</sub> and Nucleobases. <i>Springer Proceedings in Physics</i> , <b>2015</b> , 509-513	0.2	1
7	CHAPTER 10:General Trajectory Surface Hopping Method for Ultrafast Nonadiabatic Dynamics. <i>RSC Theoretical and Computational Chemistry Series</i> ,348-385	1.2	1
6	Adiabatic elimination in strong-field light-matter coupling. <i>Physical Review A</i> , <b>2020</b> , 102,	2.6	1
5	A Force Field for a Manganese-Vanadium Water Oxidation Catalyst: Redox Potentials in Solution as Showcase. <i>Catalysts</i> , <b>2021</b> , 11, 493	4	1
4	Photo-Initiated Cobalt-Catalyzed Radical Olefin Hydrogenation. <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 16978-16989	4.8	1
3	Competition between dynamic resonance and internal conversion in strong-field molecular ionization with chirped ultrafast laser pulses. <i>Physical Review A</i> , <b>2021</b> , 103,	2.6	1
2	Ultrafast photochemistry of a molybdenum carbonyl-nitrosyl complex with a triazacyclononane coligand. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 24187-24199	3.6	0
1	Laser-Induced Oxygen Formation from Carbon Dioxide. <i>Journal of Physics: Conference Series</i> , <b>2017</b> , 875, 032024	0.3	