

Enrico Tapavicza

List of Publications by Year in descending order

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28
papers

2,247
citations

394421

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501196

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docs citations

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times ranked

2397
citing authors

#	ARTICLE	IF	CITATIONS
1	TURBOMOLE: Modular program suite for <i>ab initio</i> quantum-chemical and condensed-matter simulations. <i>Journal of Chemical Physics</i> , 2020, 152, 184107.	3.0	616
2	Trajectory Surface Hopping within Linear Response Time-Dependent Density-Functional Theory. <i>Physical Review Letters</i> , 2007, 98, 023001.	7.8	324
3	Mixed time-dependent density-functional theory/classical trajectory surface hopping study of oxirane photochemistry. <i>Journal of Chemical Physics</i> , 2008, 129, 124108.	3.0	182
4	Electronic spectra from TDDFT and machine learning in chemical space. <i>Journal of Chemical Physics</i> , 2015, 143, 084111.	3.0	173
5	Ab initio non-adiabatic molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18336.	2.8	145
6	Nonadiabatic coupling vectors within linear response time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2009, 130, 124107.	3.0	114
7	Unravelling the details of vitamin D photosynthesis by non-adiabatic molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 20986.	2.8	87
8	Weakly Bonded Complexes of Aliphatic and Aromatic Carbon Compounds Described with Dispersion Corrected Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1673-1679.	5.3	66
9	Non-adiabatic dynamics using time-dependent density functional theory: Assessing the coupling strengths. <i>Computational and Theoretical Chemistry</i> , 2009, 914, 22-29.	1.5	61
10	Tuning the Efficacy of Ruthenium(II)-Arene (RAPTA) Antitumor Compounds with Fluorinated Arene Ligands. <i>Organometallics</i> , 2009, 28, 5061-5071.	2.3	61
11	Nitrogen-Containing, Light-Absorbing Oligomers Produced in Aerosol Particles Exposed to Methylglyoxal, Photolysis, and Cloud Cycling. <i>Environmental Science & Technology</i> , 2018, 52, 4061-4071.	10.0	59
12	Calculation of vibrationally resolved absorption spectra of acenes and pyrene. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21094-21103.	2.8	47
13	Direct photolysis of carbonyl compounds dissolved in cloud and fog-droplets. <i>Atmospheric Chemistry and Physics</i> , 2013, 13, 9461-9477.	4.9	44
14	Cyclohexadiene Revisited: A Time-Resolved Photoelectron Spectroscopy and <i>ab Initio</i> Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2320-2329.	2.5	42
15	Importance of Vibronic Effects in the UV-Vis Spectrum of the 7,7,8,8-Tetracyanoquinodimethane Anion. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5058-5066.	5.3	35
16	Quantum Mechanical/Molecular Mechanical (QM/MM) Car-Parrinello Simulations in Excited States. <i>Chimia</i> , 2005, 59, 493-498.	0.6	34
17	The role of tachysterol in vitamin D photosynthesis – a non-adiabatic molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 5763-5777.	2.8	27
18	Ab Initio Excited State Properties and Dynamics of a Prototype π -Bridged-Donor-Acceptor Molecule. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9595-9602.	2.5	21

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19	That Little Extra Kick: Nonadiabatic Effects in Acetaldehyde Photodissociation. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4185-4190.	4.6	21
20	First-Principles Prediction of Wavelength-Dependent Product Quantum Yields. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4758-4764.	4.6	17
21	Azologization and repurposing of a hetero-stilbene-based kinase inhibitor: towards the design of photoswitchable sirtuin inhibitors. <i>Beilstein Journal of Organic Chemistry</i> , 2019, 15, 2170-2183.	2.2	13
22	First principles theoretical spectroscopy of methylene blue: Between limitations of time-dependent density functional theory approximations and its realistic description in the solvent. <i>Journal of Chemical Physics</i> , 2021, 154, 044106.	3.0	13
23	Applicability of the Thawed Gaussian Wavepacket Dynamics to the Calculation of Vibronic Spectra of Molecules with Double-Well Potential Energy Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3065-3074.	5.3	13
24	Generating Function Approach to Single Vibronic Level Fluorescence Spectra. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6003-6009.	4.6	11
25	Tuning the photoreactivity of Z-hexatriene photoswitches by substituents – a non-adiabatic molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 24807-24820.	2.8	10
26	Elucidating an Atmospheric Brown Carbon Species – Toward Supplanting Chemical Intuition with Exhaustive Enumeration and Machine Learning. <i>Environmental Science & Technology</i> , 2021, 55, 8447-8457.	10.0	6
27	Probing the Formation and Conformational Relaxation of Previtamin D ₃ and Analogues in Solution and in Lipid Bilayers. <i>Journal of Physical Chemistry B</i> , 2021, 125, 10085-10096.	2.6	4
28	Tackling Non-Adiabatic Effects by Time-Dependent Density Functional Theory. , 2010, , .		0