Enrico Tapavicza

List of Publications by Year
in descending order

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28	2,247	394286	501076
papers	citations	19 h-index	28 g-index

34	34	34	2397
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	1.2	616
2	Trajectory Surface Hopping within Linear Response Time-Dependent Density-Functional Theory. Physical Review Letters, 2007, 98, 023001.	2.9	324
3	Mixed time-dependent density-functional theory/classical trajectory surface hopping study of oxirane photochemistry. Journal of Chemical Physics, 2008, 129, 124108.	1.2	182
4	Electronic spectra from TDDFT and machine learning in chemical space. Journal of Chemical Physics, 2015, 143, 084111.	1.2	173
5	Ab initio non-adiabatic molecular dynamics. Physical Chemistry Chemical Physics, 2013, 15, 18336.	1.3	145
6	Nonadiabatic coupling vectors within linear response time-dependent density functional theory. Journal of Chemical Physics, 2009, 130, 124107.	1.2	114
7	Unravelling the details of vitamin D photosynthesis by non-adiabatic molecular dynamics simulations. Physical Chemistry Chemical Physics, 2011, 13, 20986.	1.3	87
8	Weakly Bonded Complexes of Aliphatic and Aromatic Carbon Compounds Described with Dispersion Corrected Density Functional Theory. Journal of Chemical Theory and Computation, 2007, 3, 1673-1679.	2.3	66
9	Non-adiabatic dynamics using time-dependent density functional theory: Assessing the coupling strengths. Computational and Theoretical Chemistry, 2009, 914, 22-29.	1.5	61
10	Tuning the Efficacy of Ruthenium(II)-Arene (RAPTA) Antitumor Compounds with Fluorinated Arene Ligands. Organometallics, 2009, 28, 5061-5071.	1.1	61
11	Nitrogen-Containing, Light-Absorbing Oligomers Produced in Aerosol Particles Exposed to Methylglyoxal, Photolysis, and Cloud Cycling. Environmental Science & Technology, 2018, 52, 4061-4071.	4.6	59
12	Calculation of vibrationally resolved absorption spectra of acenes and pyrene. Physical Chemistry Chemical Physics, 2019, 21, 21094-21103.	1.3	47
13	Direct photolysis of carbonyl compounds dissolved in cloud and fog~droplets. Atmospheric Chemistry and Physics, 2013, 13, 9461-9477.	1.9	44
14	Cyclohexadiene Revisited: A Time-Resolved Photoelectron Spectroscopy and ab Initio Study. Journal of Physical Chemistry A, 2016, 120, 2320-2329.	1.1	42
15	Importance of Vibronic Effects in the UVâ€“Vis Spectrum of the 7,7,8,8-Tetracyanoquinodimethane Anion. Journal of Chemical Theory and Computation, 2016, 12, 5058-5066.	2.3	35
16	Quantum Mechanical/Molecular Mechanical (QM/MM) Car-Parrinello Simulations in Excited States. Chimia, 2005, 59, 493-498.	0.3	34
17	The role of tachysterol in vitamin D photosynthesis â€“ a non-adiabatic molecular dynamics study. Physical Chemistry Chemical Physics, 2017, 19, 5763-5777.	1.3	27
18	Ab Initio Excited State Properties and Dynamics of a Prototype Ïƒ-Bridged-Donorâ^'Acceptor Molecule. Journal of Physical Chemistry A, 2009, 113, 9595-9602.	1.1	21

#	Article	IF	Citations
19	That Little Extra Kick: Nonadiabatic Effects in Acetaldehyde Photodissociation. Journal of Physical Chemistry Letters, 2016, 7, 4185-4190.	2.1	21
20	First-Principles Prediction of Wavelength-Dependent Product Quantum Yields. Journal of Physical Chemistry Letters, 2018, 9, 4758-4764.	2.1	17
21	Azologization and repurposing of a hetero-stilbene-based kinase inhibitor: towards the design of photoswitchable sirtuin inhibitors. Beilstein Journal of Organic Chemistry, 2019, 15, 2170-2183.	1.3	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. Journal of Chemical Physics, 2021, 154, 044106.	1.2	13
23	Applicability of the Thawed Gaussian Wavepacket Dynamics to the Calculation of Vibronic Spectra of Molecules with Double-Well Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2022, 18, 3065-3074.	2.3	13
24	Generating Function Approach to Single Vibronic Level Fluorescence Spectra. Journal of Physical Chemistry Letters, 2019, 10, 6003-6009.	2.1	11
25	Tuning the photoreactivity of Z-hexatriene photoswitches by substituents â€“ a non-adiabatic molecular dynamics study. Physical Chemistry Chemical Physics, 2018, 20, 24807-24820.	1.3	10
26	Elucidating an Atmospheric Brown Carbon Speciesâ€”Toward Supplanting Chemical Intuition with Exhaustive Enumeration and Machine Learning. Environmental Science & Technology, 2021, 55, 8447-8457.	4.6	6
27	Probing the Formation and Conformational Relaxation of Previtamin D₃ and Analogues in Solution and in Lipid Bilayers. Journal of Physical Chemistry B, 2021, 125, 10085-10096.	1.2	4
28	Tackling Non-Adiabatic Effects by Time-Dependent Density Functional Theory. , 2010, , .		0