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	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
2	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
3	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
4	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
5	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	1.2	616
6	Generating Function Approach to Single Vibronic Level Fluorescence Spectra. Journal of Physical Chemistry Letters, 2019, 10, 6003-6009.	2.1	11
7	Calculation of vibrationally resolved absorption spectra of acenes and pyrene. Physical Chemistry Chemical Physics, 2019, 21, 21094-21103.	1.3	47
8	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
9	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
10	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
11	First-Principles Prediction of Wavelength-Dependent Product Quantum Yields. Journal of Physical Chemistry Letters, 2018, 9, 4758-4764.	2.1	17
12	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
13	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
14	That Little Extra Kick: Nonadiabatic Effects in Acetaldehyde Photodissociation. Journal of Physical Chemistry Letters, 2016, 7, 4185-4190.	2.1	21
15	Cyclohexadiene Revisited: A Time-Resolved Photoelectron Spectroscopy and ab Initio Study. Journal of Physical Chemistry A, 2016, 120, 2320-2329.	1.1	42
16	Electronic spectra from TDDFT and machine learning in chemical space. Journal of Chemical Physics, 2015, 143, 084111.	1.2	173
17	Ab initio non-adiabatic molecular dynamics. Physical Chemistry Chemical Physics, 2013, 15, 18336.	1.3	145
18	Direct photolysis of carbonyl compounds dissolved in cloud and fog~droplets. Atmospheric Chemistry and Physics, 2013, 13, 9461-9477.	1.9	44

#	Article	IF	Citations
19	Unravelling the details of vitamin D photosynthesis by non-adiabatic molecular dynamics simulations. Physical Chemistry Chemical Physics, 2011, 13, 20986.	1.3	87
20	Tackling Non-Adiabatic Effects by Time-Dependent Density Functional Theory. , 2010, , .		0
21	Non-adiabatic dynamics using time-dependent density functional theory: Assessing the coupling strengths. Computational and Theoretical Chemistry, 2009, 914, 22-29.	1.5	61
22	Tuning the Efficacy of Ruthenium(II)-Arene (RAPTA) Antitumor Compounds with Fluorinated Arene Ligands. Organometallics, 2009, 28, 5061-5071.	1.1	61
23	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
24	Nonadiabatic coupling vectors within linear response time-dependent density functional theory. Journal of Chemical Physics, 2009, 130, 124107.	1.2	114
25	Mixed time-dependent density-functional theory/classical trajectory surface hopping study of oxirane photochemistry. Journal of Chemical Physics, 2008, 129, 124108.	1.2	182
26	Trajectory Surface Hopping within Linear Response Time-Dependent Density-Functional Theory. Physical Review Letters, 2007, 98, 023001.	2.9	324
27	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
28	Quantum Mechanical/Molecular Mechanical (QM/MM) Car-Parrinello Simulations in Excited States. Chimia, 2005, 59, 493-498.	0.3	34