Ciro Achille Guido

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8102359/publications.pdf

Version: 2024-02-01

34	2,216	257450	361022
papers	citations	24 h-index	35 g-index

35	35	35	2702
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	On the Metric of Charge Transfer Molecular Excitations: A Simple Chemical Descriptor. Journal of Chemical Theory and Computation, 2013, 9, 3118-3126.	5.3	335
2	Practical computation of electronic excitation in solution: vertical excitation model. Chemical Science, 2011, 2, 2143.	7.4	202
3	Structures and Properties of Electronically Excited Chromophores in Solution from the Polarizable Continuum Model Coupled to the Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 3009-3020.	2.5	173
4	A fully automated implementation of VPT2 Infrared intensities. Chemical Physics Letters, 2010, 496, 157-161.	2.6	140
5	Planar vs. twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory. Physical Chemistry Chemical Physics, 2010, 12, 8016.	2.8	126
6	Benchmarking Time-Dependent Density Functional Theory for Excited State Geometries of Organic Molecules in Gas-Phase and in Solution. Journal of Chemical Theory and Computation, 2013, 9, 2209-2220.	5.3	123
7	Circularly Polarized Luminescence from Axially Chiral BODIPY DYEmers: An Experimental and Computational Study. Chemistry - A European Journal, 2016, 22, 16089-16098.	3.3	119
8	Communication: One third: A new recipe for the PBE0 paradigm. Journal of Chemical Physics, 2013, 138, 021104.	3.0	115
9	Electronic Excitations in Solution: The Interplay between State Specific Approaches and a Time-Dependent Density Functional Theory Description. Journal of Chemical Theory and Computation, 2015, 11, 5782-5790.	5.3	112
10	On the TD-DFT Accuracy in Determining Single and Double Bonds in Excited-State Structures of Organic Molecules. Journal of Physical Chemistry A, 2010, 114, 13402-13410.	2.5	76
11	An Ab Initio Description of the Excitonic Properties of LH2 and Their Temperature Dependence. Journal of Physical Chemistry B, 2016, 120, 11348-11359.	2.6	64
12	Effective electron displacements: A tool for time-dependent density functional theory computational spectroscopy. Journal of Chemical Physics, 2014, 140, 104101.	3.0	63
13	The Betheâ€“Salpeter formalism with polarisable continuum embedding: reconciling linear-response and state-specific features. Chemical Science, 2018, 9, 4430-4443.	7.4	55
14	Coupling to Charge Transfer States is the Key to Modulate the Optical Bands for Efficient Light Harvesting in Purple Bacteria. Journal of Physical Chemistry Letters, 2018, 9, 6892-6899.	4.6	55
15	The Fate of a Zwitterion in Water from ab Initio Molecular Dynamics: Monoethanolamine (MEA)-CO₂. Journal of Chemical Theory and Computation, 2013, 9, 28-32.	5.3	50
16	First-principles investigation of the double ESIPT process in a thiophene-based dye. Physical Chemistry Chemical Physics, 2019, 21, 2307-2317.	2.8	48
17	EXAT: EXcitonic analysis tool. Journal of Computational Chemistry, 2018, 39, 279-286.	3.3	37
18	Simple Protocol for Capturing Both Linear-Response and State-Specific Effects in Excited-State Calculations with Continuum Solvation Models. Journal of Chemical Theory and Computation, 2021, 17, 5155-5164.	5.3	36

#	Article	IF	Citations
19	Excited State Dipole Moments in Solution: Comparison between State-Specific and Linear-Response TD-DFT Values. Journal of Chemical Theory and Computation, 2018, 14, 1544-1553.	5.3	33
20	The role of magneticâ€“electric coupling in exciton-coupled ECD spectra: the case of bis-phenanthrenes. Chemical Communications, 2015, 51, 10498-10501.	4.1	32
21	Metrics for Molecular Electronic Excitations: A Comparison between Orbital- and Density-Based Descriptors. Journal of Physical Chemistry A, 2017, 121, 7543-7549.	2.5	32
22	Hybrid theoretical models for molecular nanoplasmonics. Journal of Chemical Physics, 2020, 153, 200901.	3.0	27
23	Excited state gradients for a state-specific continuum solvation approach: The vertical excitation model within a Lagrangian TDDFT formulation. Journal of Chemical Physics, 2017, 146, 204106.	3.0	26
24	On the description of the environment polarization response to electronic transitions. International Journal of Quantum Chemistry, 2019, 119, e25711.	2.0	25
25	Density-Dependent Formulation of Dispersionâ€“Repulsion Interactions in Hybrid Multiscale Quantum/Molecular Mechanics (QM/MM) Models. Journal of Chemical Theory and Computation, 2018, 14, 1671-1681.	5.3	24
26	Plasmon Enhanced Light Harvesting: Multiscale Modeling of the FMO Protein Coupled with Gold Nanoparticles. Journal of Physical Chemistry A, 2015, 119, 5197-5206.	2.5	18
27	Circular Dichroism and TDDFT Investigation of Chiral Fluorinated Aryl Benzyl Sulfoxides. European Journal of Organic Chemistry, 2015, 2015, 5554-5562.	2.4	14
28	Control of Coherences and Optical Responses of Pigmentâ€“Protein Complexes by Plasmonic Nanoantennae. Journal of Physical Chemistry Letters, 2016, 7, 2189-2196.	4.6	14
29	An open quantum system theory for polarizable continuum models. Journal of Chemical Physics, 2020, 152, 174114.	3.0	14
30	Calorimetric investigation of the aggregation of lithium perfluorooctanoate on poly(ethyleneglycol) oligomers in water. Thermochimica Acta, 2006, 451, 73-79.	2.7	10
31	Investigating ultrafast two-pulse experiments on single DNQDI fluorophores: a stochastic quantum approach. Physical Chemistry Chemical Physics, 2020, 22, 16734-16746.	2.8	8
32	Negative solvatochromism of pushâ€“pull biphenyl compounds: a theoretical study. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	6
33	Computational Studies of Environmental Effects and Their Interplay With Experiment. Advances in Physical Organic Chemistry, 2016, , 203-241.	0.5	2
34	Exploring the Spatial Features of Electronic Transitions in Molecular and Biomolecular Systems by Swift Electrons. Journal of Chemical Theory and Computation, 2021, 17, 2364-2373.	5.3	1