Antonio Prlj

List of Publications by Year
in descending order

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29 papers	878 citations	394286 19 h-index	501076 28 g-index
31 all docs	31 docs citations	31 times ranked	1421 citing authors

#	Article	IF	Citations
1	Calculating Photoabsorption Cross-Sections for Atmospheric Volatile Organic Compounds. ACS Earth and Space Chemistry, 2022, 6, 207-217.	1.2	14
2	Suppressing dimer formation by increasing conformational freedom in multi-carbazole thermally activated delayed fluorescence emitters. Journal of Materials Chemistry C, 2021, 9, 189-198.	2.7	25
3	Caveat when using ADC(2) for studying the photochemistry of carbonyl-containing molecules. Physical Chemistry Chemical Physics, 2021, 23, 12945-12949.	1.3	15
4	On the Theoretical Determination of Photolysis Properties for Atmospheric Volatile Organic Compounds. Journal of Physical Chemistry Letters, 2020, 11, 5418-5425.	2.1	25
5	Modulation of charge transfer by N-alkylation to control photoluminescence energy and quantum yield. Chemical Science, 2020, 11, 6990-6995.	3.7	9
6	Semiclassical Approach to Photophysics Beyond Kashaâ€™s Rule and Vibronic Spectroscopy Beyond the Condon Approximation. The Case of Azulene. Journal of Chemical Theory and Computation, 2020, 16, 2617-2626.	2.3	29
7	Direct Observation of Aggregationâ€Induced Emission Mechanism. Angewandte Chemie, 2020, 132, 15013-15019.	1.6	9
8	Direct Observation of Aggregationâ€Induced Emission Mechanism. Angewandte Chemie - International Edition, 2020, 59, 14903-14909.	7.2	85
9	Getting the Right Twist: Influence of Donorâ€“Acceptor Dihedral Angle on Exciton Kinetics and Singletâ€“Triplet Gap in Deep Blue Thermally Activated Delayed Fluorescence Emitter. Journal of Physical Chemistry C, 2019, 123, 27778-27784.	1.5	40
10	Mechanisms of fluorescence quenching in prototypical aggregation-induced emission systems: excited state dynamics with TD-DFTB. Physical Chemistry Chemical Physics, 2019, 21, 9026-9035.	1.3	28
11	Multiarm and Substituent Effects on Charge Transport of Organic Hole Transport Materials. Chemistry of Materials, 2019, 31, 6605-6614.	3.2	21
12	How does alkyl chain length modify the properties of triphenylamine-based hole transport materials?. Journal of Materials Chemistry C, 2018, 6, 960-965.	2.7	23
13	Infrared Spectroscopy as a Probe of Electronic Energy Transfer. Journal of Physical Chemistry Letters, 2018, 9, 3217-3223.	2.1	10
14	Enhancing the power conversion efficiency of dye-sensitized solar cells via molecular plasmon-like excitations. Chemical Communications, 2017, 53, 2423-2426.	2.2	6
15	Fluorescence Quenching in BODIPY Dyes: The Role of Intramolecular Interactions and Charge Transfer. Helvetica Chimica Acta, 2017, 100, e1700093.	1.0	45
16	Photochemistry of 1â€•and 2â€Naphthols and Their Water Clusters: The Role of ¹Ï€Ï€*(L_a) Mediated Hydrogen Transfer to Carbon Atoms. Chemistry - A European Journal, 2017, 23, 8244-8251.	1.7	18
17	Charge transport in highly ordered organic nanofibrils: lessons from modelling. Journal of Materials Chemistry C, 2017, 5, 350-361.	2.7	22
18	A Rising Star: Truxene as a Promising Hole Transport Material in Perovskite Solar Cells. Journal of Physical Chemistry C, 2017, 121, 21729-21739.	1.5	32

#	Article	IF	Citations
19	Low-Lying Ï€Ï€* States of Heteroaromatic Molecules: A Challenge for Excited State Methods. Journal of Chemical Theory and Computation, 2016, 12, 2652-2660.	2.3	56
20	Rationalizing fluorescence quenching in meso-BODIPY dyes. Physical Chemistry Chemical Physics, 2016, 18, 32668-32672.	1.3	48
21	How does tetraphenylethylene relax from its excited states?. Physical Chemistry Chemical Physics, 2016, 18, 11606-11609.	1.3	86
22	Intramolecular symmetry-adapted perturbation theory with a single-determinant wavefunction. Journal of Chemical Physics, 2015, 143, 224107.	1.2	19
23	Investigation of the water exchange mechanism of the Plutonyl(VI) and Uranyl(VI) ions with quantum chemical methods. Journal of Coordination Chemistry, 2015, 68, 3328-3339.	0.8	5
24	Timescales of Nâ€“H bond dissociation in pyrrole: a nonadiabatic dynamics study. Physical Chemistry Chemical Physics, 2015, 17, 19012-19020.	1.3	40
25	Excited state dynamics of thiophene and bithiophene: new insights into theoretically challenging systems. Physical Chemistry Chemical Physics, 2015, 17, 14719-14730.	1.3	57
26	Qualitatively Incorrect Features in the TDDFT Spectrum of Thiophene-Based Compounds. Journal of Physical Chemistry Letters, 2015, 6, 13-21.	2.1	62
27	Adjusting the Local Arrangement of Ï€-Stacked Oligothiophenes through Hydrogen Bonds: A Viable Route to Promote Charge Transfer. Journal of Physical Chemistry Letters, 2014, 5, 2320-2324.	2.1	22
28	Photoinduced Dynamics of Formic Acid Monomers and Dimers: The Role of the Double Hydrogen Bond. Journal of Physical Chemistry A, 2012, 116, 11467-11475.	1.1	26
29	From phosphorescence to delayed fluorescence in one step: tuning photophysical properties by quaternisation of an sp²-hybridised nitrogen atom. Journal of Materials Chemistry C, 0, , .	2.7	1