

# Antonio Prlj

## List of Publications by Year in descending order

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Version: 2024-02-01

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	How does tetraphenylethylene relax from its excited states?. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11606-11609.	1.3	86
2	Direct Observation of Aggregation-Induced Emission Mechanism. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 14903-14909.	7.2	85
3	Qualitatively Incorrect Features in the TDDFT Spectrum of Thiophene-Based Compounds. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 13-21.	2.1	62
4	Excited state dynamics of thiophene and bithiophene: new insights into theoretically challenging systems. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14719-14730.	1.3	57
5	Low-Lying $\pi^*$ States of Heteroaromatic Molecules: A Challenge for Excited State Methods. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2652-2660.	2.3	56
6	Rationalizing fluorescence quenching in meso-BODIPY dyes. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32668-32672.	1.3	48
7	Fluorescence Quenching in BODIPY Dyes: The Role of Intramolecular Interactions and Charge Transfer. <i>Helvetica Chimica Acta</i> , 2017, 100, e1700093.	1.0	45
8	Timescales of N-H bond dissociation in pyrrole: a nonadiabatic dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 19012-19020.	1.3	40
9	Getting the Right Twist: Influence of Donor-Acceptor Dihedral Angle on Exciton Kinetics and Singlet-Triplet Gap in Deep Blue Thermally Activated Delayed Fluorescence Emitter. <i>Journal of Physical Chemistry C</i> , 2019, 123, 27778-27784.	1.5	40
10	A Rising Star: Truxene as a Promising Hole Transport Material in Perovskite Solar Cells. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21729-21739.	1.5	32
11	Semiclassical Approach to Photophysics Beyond Kasha's Rule and Vibronic Spectroscopy Beyond the Condon Approximation. The Case of Azulene. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2617-2626.	2.3	29
12	Mechanisms of fluorescence quenching in prototypical aggregation-induced emission systems: excited state dynamics with TD-DFTB. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9026-9035.	1.3	28
13	Photoinduced Dynamics of Formic Acid Monomers and Dimers: The Role of the Double Hydrogen Bond. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11467-11475.	1.1	26
14	On the Theoretical Determination of Photolysis Properties for Atmospheric Volatile Organic Compounds. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 5418-5425.	2.1	25
15	Suppressing dimer formation by increasing conformational freedom in multi-carbazole thermally activated delayed fluorescence emitters. <i>Journal of Materials Chemistry C</i> , 2021, 9, 189-198.	2.7	25
16	How does alkyl chain length modify the properties of triphenylamine-based hole transport materials?. <i>Journal of Materials Chemistry C</i> , 2018, 6, 960-965.	2.7	23
17	Adjusting the Local Arrangement of $\pi$ -Stacked Oligothiophenes through Hydrogen Bonds: A Viable Route to Promote Charge Transfer. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2320-2324.	2.1	22
18	Charge transport in highly ordered organic nanofibrils: lessons from modelling. <i>Journal of Materials Chemistry C</i> , 2017, 5, 350-361.	2.7	22

#	ARTICLE	IF	CITATIONS
19	Multiam and Substituent Effects on Charge Transport of Organic Hole Transport Materials. Chemistry of Materials, 2019, 31, 6605-6614.	3.2	21
20	Intramolecular symmetry-adapted perturbation theory with a single-determinant wavefunction. Journal of Chemical Physics, 2015, 143, 224107.	1.2	19
21	Photochemistry of 1 <sup>+</sup> and 2 <sup>+</sup> Naphthols and Their Water Clusters: The Role of <sup>1</sup> L <sub>a</sub> Mediated Hydrogen Transfer to Carbon Atoms. Chemistry - A European Journal, 2017, 23, 8244-8251.	1.7	18
22	Caveat when using ADC(2) for studying the photochemistry of carbonyl-containing molecules. Physical Chemistry Chemical Physics, 2021, 23, 12945-12949.	1.3	15
23	Calculating Photoabsorption Cross-Sections for Atmospheric Volatile Organic Compounds. ACS Earth and Space Chemistry, 2022, 6, 207-217.	1.2	14
24	Infrared Spectroscopy as a Probe of Electronic Energy Transfer. Journal of Physical Chemistry Letters, 2018, 9, 3217-3223.	2.1	10
25	Modulation of charge transfer by <i>N</i> -alkylation to control photoluminescence energy and quantum yield. Chemical Science, 2020, 11, 6990-6995.	3.7	9
26	Direct Observation of Aggregation-Induced Emission Mechanism. Angewandte Chemie, 2020, 132, 15013-15019.	1.6	9
27	Enhancing the power conversion efficiency of dye-sensitized solar cells via molecular plasmon-like excitations. Chemical Communications, 2017, 53, 2423-2426.	2.2	6
28	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
29	From phosphorescence to delayed fluorescence in one step: tuning photophysical properties by quaternisation of an sp <sup>2</sup> -hybridised nitrogen atom. Journal of Materials Chemistry C, 0, , .	2.7	1