

# Merle I S Rhr

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

32  
papers

683  
citations

15  
h-index

26  
g-index

36  
ext. papers

915  
ext. citations

8.3  
avg, IF

4.5  
L-index

#	Paper	IF	Citations
32	Perspectives in Dye Chemistry: A Rational Approach toward Functional Materials by Understanding the Aggregate State. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 4500-4518	16.4	46
31	Endohedral Hydrogen Bonding Templates the Formation of a Highly Strained Covalent Organic Cage Compound*. <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 6077-6085	4.8	9
30	New theoretical methods for the exploration of functional landscapes. <i>International Journal of Quantum Chemistry</i> , <b>2021</b> , 121, e26747	2.1	
29	Isolated 2-hydroxypyrene and its dimer: a frequency- and time-resolved spectroscopic study. <i>New Journal of Chemistry</i> , <b>2021</b> , 45, 14949-14956	3.6	1
28	Energetics and optimal molecular packing for singlet fission in BN-doped perylenes: electronic adiabatic state basis screening. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 16525-16536	3.6	1
27	Impact of substituents on molecular properties and catalytic activities of trinuclear Ru macrocycles in water oxidation. <i>Chemical Science</i> , <b>2020</b> , 11, 7654-7664	9.4	9
26	Control of self-assembly pathways toward conglomerate and racemic supramolecular polymers. <i>Nature Communications</i> , <b>2020</b> , 11, 5460	17.4	16
25	Tuning phenoxy-substituted diketopyrrolopyrroles from quinoidal to biradical ground states through (hetero-)aromatic linkers. <i>Chemical Science</i> , <b>2020</b> , 12, 793-802	9.4	8
24	Spectral and Structural Variations of Biomimetic Light-Harvesting Nanotubes. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 2715-2724	6.4	16
23	metaFALCON: A Program Package for Automatic Sampling of Conical Intersection Seams Using Multistate Metadynamics. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 3450-3460	6.4	14
22	Dynamic exciton localisation in a pyrene-BODIPY-pyrene dye conjugate. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 9013-9025	3.6	7
21	Supramolecular Polymorphism in One-Dimensional Self-Assembly by Kinetic Pathway Control. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 6092-6107	16.4	102
20	Metadynamics for automatic sampling of quantum property manifolds: exploration of molecular biradicality landscapes. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 24716-24722	3.6	2
19	A Self-Assembled Unit Comprising 12 Squaraine Dyes Built Up from Two Star-Shaped Hexasquarainyl-Benzene Molecules. <i>Chemistry - A European Journal</i> , <b>2019</b> , 25, 2831-2839	4.8	5
18	Exciton Dynamics from Strong to Weak Coupling Limit Illustrated on a Series of Squaraine Dimers. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 8082-8093	3.8	33
17	Isolation of diborenes and their 90°-twisted diradical congeners. <i>Nature Communications</i> , <b>2018</b> , 9, 1197	17.4	41
16	Multistate metadynamics for automatic exploration of conical intersections. <i>Physical Review A</i> , <b>2018</b> , 97,	2.6	6

15	The mechanism of excimer formation: an experimental and theoretical study on the pyrene dimer. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 25002-25015	3.6	76
14	A Crystalline $\pi$ Stack Containing Five Stereoisomers: Insights into Conformational Isomorphism, Chirality Inversion, and Disorder. <i>Angewandte Chemie</i> , <b>2017</b> , 129, 11936-11940	3.6	12
13	A Crystalline $\pi$ Stack Containing Five Stereoisomers: Insights into Conformational Isomorphism, Chirality Inversion, and Disorder. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 11774-11778	16.4	24
12	Cooperative water oxidation catalysis in a series of trinuclear metallosupramolecular ruthenium macrocycles. <i>Energy and Environmental Science</i> , <b>2017</b> , 10, 2137-2153	35.4	27
11	First-principles simulation of light propagation and exciton dynamics in metal cluster nanostructures. <i>Applied Physics B: Lasers and Optics</i> , <b>2016</b> , 122, 1	1.9	2
10	Excitonic Properties of Ordered Metal Nanocluster Arrays: 2D Silver Clusters at Multiporphyrin Templates. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 4465-72	2.8	5
9	Vibrationally resolved optical spectra and ultrafast electronic relaxation dynamics of diamantane. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 8701-9	3.6	5
8	Laser-induced fluorescence of free diamondoid molecules. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 4739-49	3.6	15
7	Energy Transfer Between Squaraine Polymer Sections: From Helix to Zigzag and All the Way Back. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 7851-61	16.4	41
6	Site-dependence of van der Waals interaction explains exciton spectra of double-walled tubular J-aggregates. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 6741-7	3.6	36
5	Tuning Structural and Optical Properties of Thiolate-Protected Silver Clusters by Formation of a Silver Core with Confined Electrons. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 14824-14831	3.8	32
4	Nonlinear absorption dynamics using field-induced surface hopping: zinc porphyrin in water. <i>ChemPhysChem</i> , <b>2013</b> , 14, 1377-86	3.2	14
3	Synthesis and Spectroscopic Characterization of Diphenylargentate, $[(C_6H_5)_2Ag](.)$ . <i>Journal of Physical Chemistry Letters</i> , <b>2012</b> , 3, 1197-201	6.4	15
2	Gas-Phase Synthesis and Vibronic Action Spectroscopy of $Ag_2H^+$ . <i>Journal of Physical Chemistry Letters</i> , <b>2011</b> , 2, 548-552	6.4	19
1	Structural and photochemical properties of organosilver reactive intermediates $MeAg_2(+)$ and $PhAg_2(+)$ . <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 9120-7	2.8	23