

# Merle I S RÃ¶hr

## List of Publications by Year in descending order

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34  
papers

1,095  
citations

471061

17  
h-index

414034

32  
g-index

36  
all docs

36  
docs citations

36  
times ranked

1448  
citing authors

#	ARTICLE	IF	CITATIONS
1	Supramolecular Polymorphism in One-Dimensional Self-Assembly by Kinetic Pathway Control. <i>Journal of the American Chemical Society</i> , 2019, 141, 6092-6107.	6.6	194
2	Perspectives in Dye Chemistry: A Rational Approach toward Functional Materials by Understanding the Aggregate State. <i>Journal of the American Chemical Society</i> , 2021, 143, 4500-4518.	6.6	149
3	The mechanism of excimer formation: an experimental and theoretical study on the pyrene dimer. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 25002-25015.	1.3	119
4	Isolation of diborenes and their 90°-twisted diradical congeners. <i>Nature Communications</i> , 2018, 9, 1197.	5.8	62
5	Energy Transfer Between Squaraine Polymer Sections: From <i>Helix</i> to <i>Zigzag</i> and All the Way Back. <i>Journal of the American Chemical Society</i> , 2015, 137, 7851-7861.	6.6	50
6	Exciton Dynamics from Strong to Weak Coupling Limit Illustrated on a Series of Squaraine Dimers. <i>Journal of Physical Chemistry C</i> , 2018, 122, 8082-8093.	1.5	49
7	Site-dependence of van der Waals interaction explains exciton spectra of double-walled tubular J-aggregates. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6741-6747.	1.3	41
8	Control of self-assembly pathways toward conglomerate and racemic supramolecular polymers. <i>Nature Communications</i> , 2020, 11, 5460.	5.8	41
9	Cooperative water oxidation catalysis in a series of trinuclear metallosupramolecular ruthenium macrocycles. <i>Energy and Environmental Science</i> , 2017, 10, 2137-2153.	15.6	40
10	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> , 2013, 117, 14824-14831.	1.5	34
11	A Crystalline $\pi$ -Stack Containing Five Stereoisomers: Insights into Conformational Isomorphism, Chirality Inversion, and Disorder. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 11774-11778.	7.2	34
12	Supramolecular Approaches to Improve the Performance of Ruthenium-Based Water Oxidation Catalysts. <i>Advanced Energy Materials</i> , 2017, 7, 1602939.	10.2	26
13	Structural and Photochemical Properties of Organosilver Reactive Intermediates $\text{MeAg}_2^+$ and $\text{PhAg}_2^+$ . <i>Journal of Physical Chemistry A</i> , 2011, 115, 9120-9127.	1.1	24
14	Laser-induced fluorescence of free diamondoid molecules. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4739-4749.	1.3	20
15	Spectral and Structural Variations of Biomimetic Light-Harvesting Nanotubes. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2715-2724.	2.1	20
16	Tuning phenoxyl-substituted diketopyrrolopyrroles from quinoidal to biradical ground states through (hetero-)aromatic linkers. <i>Chemical Science</i> , 2021, 12, 793-802.	3.7	20
17	Gas-Phase Synthesis and Vibronic Action Spectroscopy of $\text{Ag}_2\text{H}^+$ . <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 548-552.	2.1	19
18	metaFALCON: A Program Package for Automatic Sampling of Conical Intersection Seams Using Multistate Metadynamics. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3450-3460.	2.3	19

#	ARTICLE	IF	CITATIONS
19	Endohedral Hydrogen Bonding Templates the Formation of a Highly Strained Covalent Organic Cage Compound**. Chemistry - A European Journal, 2021, 27, 6077-6085.	1.7	17
20	Synthesis and Spectroscopic Characterization of Diphenylargentate, $[(C_6H_5)_2Ag]^{2-}$ . Journal of Physical Chemistry Letters, 2012, 3, 1197-1201.	2.1	16
21	Nonlinear Absorption Dynamics Using Field-Induced Surface Hopping: Zinc Porphyrin in Water. ChemPhysChem, 2013, 14, 1377-1386.	1.0	16
22	A Crystalline $\pi$ - $\pi$ Stack Containing Five Stereoisomers: Insights into Conformational Isomorphism, Chirality Inversion, and Disorder. Angewandte Chemie, 2017, 129, 11936-11940.	1.6	15
23	Impact of substituents on molecular properties and catalytic activities of trinuclear Ru macrocycles in water oxidation. Chemical Science, 2020, 11, 7654-7664.	3.7	15
24	Dynamic exciton localisation in a pyrene-BODIPY-pyrene dye conjugate. Physical Chemistry Chemical Physics, 2019, 21, 9013-9025.	1.3	13
25	Multistate metadynamics for automatic exploration of conical intersections. Physical Review A, 2018, 97, .	1.0	9
26	Excitonic Properties of Ordered Metal Nanocluster Arrays: 2D Silver Clusters at Multiporphyrin Templates. Journal of Physical Chemistry A, 2016, 120, 4465-4472.	1.1	7
27	Vibrationally resolved optical spectra and ultrafast electronic relaxation dynamics of diamantane. Physical Chemistry Chemical Physics, 2016, 18, 8701-8709.	1.3	7
28	A Self-Assembled Unit Comprising 12 Squaraine Dyes Built Up from Two Star-Shaped Hexasquarainyl-Benzene Molecules. Chemistry - A European Journal, 2019, 25, 2831-2839.	1.7	6
29	Energetics and optimal molecular packing for singlet fission in BN-doped perylenes: electronic adiabatic state basis screening. Physical Chemistry Chemical Physics, 2021, 23, 16525-16536.	1.3	6
30	Isolated 2-hydroxypyrene and its dimer: a frequency- and time-resolved spectroscopic study. New Journal of Chemistry, 2021, 45, 14949-14956.	1.4	3
31	First-principles simulation of light propagation and exciton dynamics in metal cluster nanostructures. Applied Physics B: Lasers and Optics, 2016, 122, 1.	1.1	2
32	Metadynamics for automatic sampling of quantum property manifolds: exploration of molecular biradicality landscapes. Physical Chemistry Chemical Physics, 2019, 21, 24716-24722.	1.3	2
33	Water Oxidation Catalysts: Supramolecular Approaches to Improve the Performance of Ruthenium-Based Water Oxidation Catalysts (Adv. Energy Mater. 16/2017). Advanced Energy Materials, 2017, 7, .	10.2	0
34	New theoretical methods for the exploration of functional landscapes. International Journal of Quantum Chemistry, 2021, 121, e26747.	1.0	0