Julien Guthmuller

List of Publications by Year
in descending order

33 papers	1,327 citations	331670 21 h-index	361022 35 g-index
39 all docs	39 docs citations	39 times ranked	1384 citing authors

#	Article	IF	Citations
1	Lightâ€Driven Multiâ€Charge Separation in a Pushâ€Pull Rutheniumâ€Based Photosensitizer â€“ Assessed by RASSCF and TDDFT Simulations. ChemPhotoChem, 2022, 6, .	3.0	4
2	Sum-over-state expressions including second-order Herzbergâ€“Teller effects for the calculation of absorption and resonance Raman intensities. Journal of Chemical Physics, 2021, 155, 084107.	3.0	2
3	Radiative lifetime of a BODIPY dye as calculated by TDDFT and EOM-CCSD methods: solvent and vibronic effects. Physical Chemistry Chemical Physics, 2021, 23, 26324-26335.	2.8	11
4	Synthesis and hydrogen evolving catalysis of a panchromatic photochemical molecular device. Sustainable Energy and Fuels, 2020, 4, 619-624.	4.9	9
5	Effects of Bromine Doping on the Structural Properties and Band Gap of CH₃NH₃Pb(I_{1â€“x}Br_x)₃ Perovskite. ACS Omega, 2020, 5, 26946-26953.	3.5	15
6	Influence of Orientational Disorder on the Optical Absorption Properties of the Hybrid Metalâ€Halide Perovskite CH₃NH₃PbI₃. ChemPhysChem, 2019, 20, 3228-3237.	2.1	2
7	Effect of the Catalytic Center on the Electron Transfer Dynamics in Hydrogen-Evolving Ruthenium-Based Photocatalysts Investigated by Theoretical Calculations. Journal of Physical Chemistry C, 2019, 123, 16003-16013.	3.1	15
8	Excited state properties of a series of molecular photocatalysts investigated by time dependent density functional theory. Physical Chemistry Chemical Physics, 2019, 21, 9052-9060.	2.8	12
9	The role of Herzberg-Teller effects on the resonance Raman spectrum of trans-porphycene investigated by time dependent density functional theory. Journal of Chemical Physics, 2018, 148, 124107.	3.0	7
10	Theoretical Investigation of the Electronâ€Transfer Dynamics and Photodegradation Pathways in a Hydrogenâ€Evolving Rutheniumâ€“Palladium Photocatalyst. Chemistry - A European Journal, 2018, 24, 11166-11176.	3.3	12
11	Theoretical Assessment of Excited State Gradients and Resonance Raman Intensities for the Azobenzene Molecule. Journal of Chemical Theory and Computation, 2017, 13, 1263-1274.	5.3	26
12	Comparison of simplified sum-over-state expressions to calculate resonance Raman intensities including Franck-Condon and Herzberg-Teller effects. Journal of Chemical Physics, 2016, 144, 064106.	3.0	35
13	Synthesis and characterization of ruthenium and rhenium dyes with phosphonate anchoring groups. Dalton Transactions, 2016, 45, 9216-9228.	3.3	27
14	Electronic state spectroscopy by high-resolution vacuum ultraviolet photoabsorption, He(I) photoelectron spectroscopy and ab initio calculations of ethyl acetate. European Physical Journal D, 2016, 70, 1.	1.3	5
15	Ï€-Stacking attraction vs. electrostatic repulsion: competing supramolecular interactions in a tpphz-bridged Ru(<scp>ii</scp>)/Au(<scp>iii</scp>) complex. Dalton Transactions, 2016, 45, 12846-12853.	3.3	7
16	CLICK 'n' Sleep: Lightâ€Switch Behavior of Triazoleâ€Containing Tris(bipyridyl)ruthenium Complexes. European Journal of Inorganic Chemistry, 2016, 2016, 4958-4963.	2.0	7
17	Optimization of Hydrogenâ€Evolving Photochemical Molecular Devices. Angewandte Chemie - International Edition, 2015, 54, 6627-6631.	13.8	96
18	Palladium versus Platinum: The Metal in the Catalytic Center of a Molecular Photocatalyst Determines the Mechanism of the Hydrogen Production with Visible Light. Angewandte Chemie - International Edition, 2015, 54, 5044-5048.	13.8	112

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19	Frontispiece: Palladium versus Platinum: The Metal in the Catalytic Center of a Molecular Photocatalyst Determines the Mechanism of the Hydrogen Production with Visible Light. Angewandte Chemie - International Edition, 2015, 54, .	13.8	0
20	Ultrafast Intramolecular Relaxation and Waveâ€Packet Motion in a Rutheniumâ€Based Supramolecular Photocatalyst. Chemistry - A European Journal, 2015, 21, 7668-7674.	3.3	24
21	Photophysics of Ru(II) Dyads Derived from Pyrenyl-Substitued Imidazo[4,5-f][1,10]phenanthroline Ligands. Journal of Physical Chemistry A, 2015, 119, 3986-3994.	2.5	34
22	Resonance-Raman spectro-electrochemistry of intermediates in molecular artificial photosynthesis of bimetallic complexes. Chemical Communications, 2014, 50, 5227.	4.1	48
23	Redox State Sensitive Spectroscopy of the Model Compound [(H-dcbpy)₂Ru^{II}(NCS)₂]^{2â€“} (dcbpy =) Tj ETQq1 1 0.784314 rgBT /Overlock 10	3.3	1
24	An Assessment of RASSCF and TDDFT Energies and Gradients on an Organic Donorâ€“Acceptor Dye Assisted by Resonance Raman Spectroscopy. Journal of Chemical Theory and Computation, 2013, 9, 543-554.	5.3	38
25	Analysis and characterization of coordination compounds by resonance Raman spectroscopy. Coordination Chemistry Reviews, 2012, 256, 1479-1508.	18.8	95
26	A Novel Ru(II) Polypyridine Black Dye Investigated by Resonance Raman Spectroscopy and TDDFT Calculations. Journal of Physical Chemistry C, 2012, 116, 19968-19977.	3.1	30
27	Assessment of TD-DFT and CC2 Methods for the Calculation of Resonance Raman Intensities: Application to o-Nitrophenol. Journal of Chemical Theory and Computation, 2011, 7, 1082-1089.	5.3	34
28	Protonation effects on the resonance Raman properties of a novel (terpyridine)Ru(4H-imidazole) complex: an experimental and theoretical case study. Physical Chemistry Chemical Physics, 2011, 13, 15580.	2.8	54
29	Photochemical Fate: The First Step Determines Efficiency of H₂ Formation with a Supramolecular Photocatalyst. Angewandte Chemie - International Edition, 2010, 49, 3981-3984.	13.8	162
30	Simulation of the resonance Raman intensities of a rutheniumâ€“palladium photocatalyst by time dependent density functional theory. Physical Chemistry Chemical Physics, 2010, 12, 14812.	2.8	47
31	Multimode simulation of dimer absorption spectra from first principles calculations: Application to the 3,4,9,10-perylenetetracarboxylic diimide dimer. Journal of Chemical Physics, 2009, 131, 154302.	3.0	50
32	Resonance Raman Scattering of Rhodamine 6G as Calculated by Time-Dependent Density Functional Theory:â€‰ Vibronic and Solvent Effects. Journal of Physical Chemistry A, 2008, 112, 3215-3223.	2.5	87
33	Time dependent density functional theory investigation of the resonance Raman properties of the julolidinemalononitrile push-pull chromophore in various solvents. Journal of Chemical Physics, 2007, 127, 164507.	3.0	93