Thibaud Etienne

List of Publications by Year
in descending order

26	1,318	516215 16	642321 23
papers	citations	h-index	g-index

26	26	26	1972
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Activity-Based Photosensitizers with Optimized Triplet State Characteristics Toward Cancer Cell Selective and Image Guided Photodynamic Therapy. ACS Applied Bio Materials, 2022, 5, 2754-2767.	2.3	5
2	A comprehensive, selfâ€contained derivation of the oneâ€body density matrices from singleâ€reference excitedâ€state calculation methods using the equationâ€ofâ€motion formalism. International Journal of Quantum Chemistry, 2020, 120, e26110.	1.0	3
3	Diagnosis of two evaluation paths to density-based descriptors of molecular electronic transitions. Advances in Quantum Chemistry, 2019, 79, 289-310.	0.4	0
4	Charge Separation. , 2019, , 121-170.		1
5	Dynamical Rashba Band Splitting in Hybrid Perovskites Modeled by Local Electric Fields. Journal of Physical Chemistry C, 2018, 122, 124-132.	1.5	8
6	Rashba Band Splitting in Organohalide Lead Perovskites: Bulk and Surface Effects. Journal of Physical Chemistry Letters, 2017, 8, 2247-2252.	2.1	101
7	Vibronic properties of para-polyphenylene ethynylenes: TD-DFT insights. Journal of Chemical Physics, 2017, 146, 164303.	1.2	10
8	Unveiling the nature of post-linear response Z-vector method for time-dependent density functional theory. Journal of Chemical Physics, 2017, 147, 024108.	1.2	21
9	Fluorene-imidazole dyes excited states from first-principles calculationsâ€"Topological insights. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	16
10	Dynamical Origin of the Rashba Effect in Organohalide Lead Perovskites: A Key to Suppressed Carrier Recombination in Perovskite Solar Cells?. Journal of Physical Chemistry Letters, 2016, 7, 1638-1645.	2.1	278
11	A new record excited state ³MLCT lifetime for metalorganic iron(<scp>ii</scp>) complexes. Physical Chemistry Chemical Physics, 2016, 18, 12550-12556.	1.3	132
12	Structural and electronic properties of dye-sensitized TiO₂ for solar cell applications: from single molecules to self-assembled monolayers. Journal of Materials Chemistry C, 2016, 4, 4346-4373.	2.7	46
13	Transition matrices and orbitals from reduced density matrix theory. Journal of Chemical Physics, 2015, 142, 244103.	1.2	48
14	Probing the Locality of Excited States with Linear Algebra. Journal of Chemical Theory and Computation, 2015, 11, 1692-1699.	2.3	35
15	An Ironâ€Based Photosensitizer with Extended Excitedâ€State Lifetime: Photophysical and Photovoltaic Properties. European Journal of Inorganic Chemistry, 2015, 2015, 2469-2477.	1.0	124
16	2,5-Dithienylpyrrole (DTP) as a donor component in DTPâ€"Ïâ€"A organic sensitizers: photophysical and photovoltaic properties. RSC Advances, 2015, 5, 4041-4050.	1.7	16
17	Heteroleptic Pyridylâ€Carbene Iron Complexes with Tuneable Electronic Properties. European Journal of Inorganic Chemistry, 2014, 2014, 3747-3753.	1.0	59
18	Theoretical computation of Betain B30 solvatochromism using aÂPolarizable Continuum Model. Dyes and Pigments, 2014, 100, 24-31.	2.0	31

#	Article	IF	Citations
19	QM/MM modeling of Harmane cation fluorescence spectrum in water solution and interacting with DNA. Computational and Theoretical Chemistry, 2014, 1040-1041, 367-372.	1.1	20
20	All-organic chromophores for dye-sensitized solar cells: A theoretical study on aggregation. Dyes and Pigments, 2014, 101, 203-211.	2.0	22
21	QM/MM calculation of absorption spectra of complex systems: The case of human serum albumin. Computational and Theoretical Chemistry, 2014, 1040-1041, 360-366.	1.1	12
22	Toward a Quantitative Assessment of Electronic Transitionsâ€™ Charge-Transfer Character. Journal of Chemical Theory and Computation, 2014, 10, 3896-3905.	2.3	139
23	New Insight into the Topology of Excited States through Detachment/Attachment Density Matrices-Based Centroids of Charge. Journal of Chemical Theory and Computation, 2014, 10, 3906-3914.	2.3	121
24	Detection of Nitroaromatic Explosives Based on Fluorescence Quenching of Silafluorene- and Silole-Containing Polymers: A Time-Dependent Density Functional Theory Study. Journal of Physical Chemistry C, 2014, 118, 23946-23953.	1.5	27
25	A QM/MM Study of the Absorption Spectrum of Harmane in Water Solution and Interacting with DNA: The Crucial Role of Dynamic Effects. Journal of Physical Chemistry B, 2013, 117, 4973-4980.	1.2	42
26	Theoretical Insights into the Topology of Molecular Excitons from Single-Reference Excited States Calculation Methods. , 0, , .		1