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	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
2	Toward a Quantitative Assessment of Electronic Transitionsâ€™ Charge-Transfer Character. Journal of Chemical Theory and Computation, 2014, 10, 3896-3905.	2.3	139
3	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
4	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
5	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
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	Heteroleptic Pyridylâ€Carbene Iron Complexes with Tuneable Electronic Properties. European Journal of Inorganic Chemistry, 2014, 2014, 3747-3753.	1.0	59
8	Transition matrices and orbitals from reduced density matrix theory. Journal of Chemical Physics, 2015, 142, 244103.	1.2	48
9	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
10	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
11	Probing the Locality of Excited States with Linear Algebra. Journal of Chemical Theory and Computation, 2015, 11, 1692-1699.	2.3	35
12	Theoretical computation of Betain B30 solvatochromism using aÂPolarizable Continuum Model. Dyes and Pigments, 2014, 100, 24-31.	2.0	31
13	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
14	All-organic chromophores for dye-sensitized solar cells: A theoretical study on aggregation. Dyes and Pigments, 2014, 101, 203-211.	2.0	22
15	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
16	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
17	2,5-Dithienylpyrrole (DTP) as a donor component in DTPâ€“Ï€â€“A organic sensitizers: photophysical and photovoltaic properties. RSC Advances, 2015, 5, 4041-4050.	1.7	16
18	Fluorene-imidazole dyes excited states from first-principles calculationsâ€”Topological insights. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	16

#	Article	IF	Citations
19	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
20	Vibronic properties of para-polyphenylene ethynylenes: TD-DFT insights. Journal of Chemical Physics, 2017, 146, 164303.	1.2	10
21	Dynamical Rashba Band Splitting in Hybrid Perovskites Modeled by Local Electric Fields. Journal of Physical Chemistry C, 2018, 122, 124-132.	1.5	8
22	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
23	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
24	Theoretical Insights into the Topology of Molecular Excitons from Single-Reference Excited States Calculation Methods. , 0, , .		1
25	Charge Separation. , 2019, , 121-170.		1
26	Diagnosis of two evaluation paths to density-based descriptors of molecular electronic transitions. Advances in Quantum Chemistry, 2019, 79, 289-310.	0.4	0