Tangui Le Bahers

List of Publications by Year
in descending order

71 papers	4,135 citations	159525 30 h-index	110317 64 g-index
71 all docs	71 docs citations	71 times ranked	5304 citing authors

#	Article	IF	Citations
1	Electronic structures of the MoS₂/TiO₂(anatase) heterojunction: influence of physical and chemical modifications at the 2D- or 1D-interfaces. Physical Chemistry Chemical Physics, 2022, 24, 2646-2655.	1.3	6
2	Sensitive 1,1-dicyanovinyl push-pull dye for primary amine sensing in solution by fluorescence. Dyes and Pigments, 2022, 202, 110258.	2.0	9
3	The structural origin of the efficient photochromism in natural minerals. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	8
4	Thiochromenocarbazole imide: a new organic dye with first utility in large area flexible electroluminescent devices. Materials Chemistry Frontiers, 2022, 6, 1912-1919.	3.2	6
5	Ïƒâ€Conjugation and Hâ€Bondâ€Directed Supramolecular Selfâ€Assembly: Key Features for Efficient Longâ€Lived Room Temperature Phosphorescent Organic Molecular Crystals. Angewandte Chemie - International Edition, 2021, 60, 2446-2454.	7.2	29
6	Ïƒâ€Conjugation and Hâ€Bondâ€Directed Supramolecular Selfâ€Assembly: Key Features for Efficient Longâ€Lived Room Temperature Phosphorescent Organic Molecular Crystals. Angewandte Chemie, 2021, 133, 2476-2484.	1.6	9
7	Investigation of the K₄[Fe(CN)₆]-Mediated Mono- and Bis-Palladium-Catalyzed Cyanation of the Benzothioxanthene Core. Journal of Organic Chemistry, 2021, 86, 5901-5907.	1.7	6
8	Spin-orbital coupling and slow phonon effects enabled persistent photoluminescence in organic crystal under isomer doping. Nature Communications, 2021, 12, 3485.	5.8	8
9	Detection of Xâ€Ray Doses with Colorâ€Changing Hackmanites: Mechanism and Application. Advanced Optical Materials, 2021, 9, 2100762.	3.6	12
10	2D MoO_{3â€“x}S_x/MoS₂van der Waals Assembly: A Tunable Heterojunction with Attractive Properties for Photocatalysis. ACS Applied Materials & Interfaces, 2021, 13, 36465-36474.	4.0	29
11	Exploring the Concept of Dimerization-Induced Intersystem Crossing: At the Origins of Spinâ€“Orbit Coupling Selection Rules. Journal of Physical Chemistry B, 2021, 125, 8572-8580.	1.2	8
12	Phosphine-based push-pull AIE fluorophores: Synthesis, photophysical properties, and TD-DFT studies. Dyes and Pigments, 2021, 193, 109485.	2.0	1
13	What does graphitic carbon nitride really look like?. Physical Chemistry Chemical Physics, 2021, 23, 2853-2859.	1.3	12
14	Light-inducedin situchemical activation of a fluorescent probe for monitoring intracellular G-quadruplex structures. Nanoscale, 2021, 13, 13795-13808.	2.8	11
15	Tuning Excited-State Properties of [2.2]Paracyclophane-Based Antennas to Ensure Efficient Sensitization of Lanthanide Ions or Singlet Oxygen Generation. Inorganic Chemistry, 2021, 60, 16194-16203.	1.9	1
16	Hackmaniteâ€”The Natural Glow-in-the-Dark Material. Chemistry of Materials, 2020, 32, 8895-8905.	3.2	17
17	Two-Photon Absorbing AIEgens: Influence of Stereoconfiguration on Their Crystallinity and Spectroscopic Properties and Applications in Bioimaging. ACS Applied Materials & Interfaces, 2020, 12, 55157-55168.	4.0	12
18	2D hostâ€“guest supramolecular chemistry for an on-monolayer graphene emitting platform. Materials Horizons, 2020, 7, 2741-2748.	6.4	3

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19	On the understanding of the optoelectronic properties of S-doped MoO₃ and O-doped MoS₂ bulk systems: a DFT perspective. Journal of Materials Chemistry C, 2020, 8, 9064-9074.	2.7	44
20	Two-sites are better than one: revisiting the OER mechanism on CoOOH by DFT with electrode polarization. Physical Chemistry Chemical Physics, 2020, 22, 7031-7038.	1.3	45
21	Theoretical and experimental investigation on the intersystem crossing kinetics in benzothioxanthene imide luminophores, and their dependence on substituent effects. Physical Chemistry Chemical Physics, 2020, 22, 12373-12381.	1.3	11
22	On the Spectroscopic Modeling of Localized Defects in Sodalites by TD-DFT. Journal of Physical Chemistry C, 2020, 124, 8949-8957.	1.5	15
23	Catalytic consequences of ultrafine Pt clusters supported on SrTiO3 for photocatalytic overall water splitting. Journal of Catalysis, 2019, 376, 180-190.	3.1	67
24	Full in silico DFT characterization of lanthanum and yttrium based oxynitride semiconductors for solar fuels. Journal of Materials Chemistry C, 2019, 7, 1612-1621.	2.7	11
25	Combined theoretical and experimental characterizations of semiconductors for photoelectrocatalytic applications. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2019, 40, 212-233.	5.6	29
26	A â€œMultiâ€Heavyâ€Atomâ€•Approach toward Biphotonic Photosensitizers with Improved Singletâ€Oxygen Generation Properties. Chemistry - A European Journal, 2019, 25, 9026-9034.	1.7	34
27	Optoelectronic Structure and Photocatalytic Applications of Na(Bi,La)S2 Solid Solutions with Tunable Band Gaps. Chemistry of Materials, 2019, 31, 3211-3220.	3.2	13
28	Solar UV index and UV dose determination with photochromic hackmanites: from the assessment of the fundamental properties to the device. Materials Horizons, 2018, 5, 569-576.	6.4	28
29	A combined theoretical and experimental investigation on the influence of the bromine substitution pattern on the photophysics of conjugated organic chromophores. Physical Chemistry Chemical Physics, 2018, 20, 3768-3783.	1.3	17
30	Diffusion Kinetics of Gold and Copper Atoms on Pristine and Reduced Rutile TiO₂ (110) Surfaces. Journal of Physical Chemistry C, 2018, 122, 3824-3837.	1.5	12
31	Photophysical insights on the influence of excited states reorganization processes on the visible and near infra-red luminescence of two-photon quadrupolar chromophores. Dyes and Pigments, 2018, 159, 352-366.	2.0	6
32	Contribution of electrolyte in nanoscale electrolysis of pure and buffered water by particulate photocatalysis. Sustainable Energy and Fuels, 2018, 2, 2044-2052.	2.5	18
33	Shining Light on Carbon Nitrides: Leveraging Temperature To Understand Optical Gap Variations. Chemistry of Materials, 2018, 30, 4253-4262.	3.2	28
34	Challenges in calculating the bandgap of triazine-based carbon nitride structures. Journal of Materials Chemistry A, 2017, 5, 5115-5122.	5.2	34
35	Photophysical Properties of SrTaO₂N Thin Films and Influence of Anion Ordering: A Joint Theoretical and Experimental Investigation. Chemistry of Materials, 2017, 29, 3989-3998.	3.2	37
36	Ab initio assessment of Bi_{1â^'x}RE_xCuOS (RE = La, Gd, Y, Lu) solid solutions as a semiconductor for photochemical water splitting. Physical Chemistry Chemical Physics, 2017, 19, 12321-12330.	1.3	21

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37	Modeling the Photochromism of S-Doped Sodalites Using DFT, TD-DFT, and SAC-CI Methods. Inorganic Chemistry, 2017, 56, 414-423.	1.9	18
38	Bismuth Silver Oxysulfide for Photoconversion Applications: Structural and Optoelectronic Properties. Chemistry of Materials, 2017, 29, 8679-8689.	3.2	28
39	Enhanced Kinetics of Hole Transfer and Electrocatalysis during Photocatalytic Oxygen Evolution by Cocatalyst Tuning. ACS Catalysis, 2016, 6, 4117-4126.	5.5	48
40	Structure of Titanâ€™s evaporites. Icarus, 2016, 270, 41-56.	1.1	32
41	DFT Perspective on the Thermochemistry of Carbon Nitride Synthesis. Journal of Physical Chemistry C, 2016, 120, 24542-24550.	1.5	21
42	How Should Iron and Titanium be Combined in Oxides to Improve Photoelectrochemical Properties?. Journal of Physical Chemistry C, 2016, 120, 24521-24532.	1.5	35
43	Carbazole-Substituted Iridium Complex as a Solid State Emitter for Two-Photon Intravital Imaging. Inorganic Chemistry, 2016, 55, 9586-9595.	1.9	18
44	Characterization and charge transfer properties of organic BODIPY dyes integrated in TiO₂nanotube based dye-sensitized solar cells. RSC Advances, 2016, 6, 91529-91540.	1.7	17
45	A Fluorescent Polymer Probe with High Selectivity toward Vascular Endothelial Cells for and beyond Noninvasive Two-Photon Intravital Imaging of Brain Vasculature. ACS Applied Materials & Interfaces, 2016, 8, 17047-17059.	4.0	20
46	Assembly of Ferrocene Molecules on Metal Surfaces Revisited. Journal of Physical Chemistry Letters, 2015, 6, 395-400.	2.1	41
47	Scrutinizing individual CoTPP molecule adsorbed on coinage metal surfaces from the interplay of STM experiment and theory. Surface Science, 2015, 635, 108-114.	0.8	12
48	Assessing the Use of BiCuOS for Photovoltaic Application: From DFT to Macroscopic Simulation. Journal of Physical Chemistry C, 2015, 119, 17585-17595.	1.5	31
49	Exploring excited states using Time Dependent Density Functional Theory and density-based indexes. Coordination Chemistry Reviews, 2015, 304-305, 166-178.	9.5	118
50	Electronic structure and photocatalytic activity of wurtzite Cuâ€“Gaâ€“S nanocrystals and their Zn substitution. Journal of Materials Chemistry A, 2015, 3, 8896-8904.	5.2	33
51	Relationship between Carbon Nitride Structure and Exciton Binding Energies: A DFT Perspective. Journal of Physical Chemistry C, 2015, 119, 25188-25196.	1.5	104
52	Dendritic Tip-on Polytriazine-Based Carbon Nitride Photocatalyst with High Hydrogen Evolution Activity. Chemistry of Materials, 2015, 27, 8237-8247.	3.2	140
53	Electronic properties of PbX₃CH₃NH₃(X = Cl, Br, I) compounds for photovoltaic and photocatalytic applications. Physical Chemistry Chemical Physics, 2015, 17, 2199-2209.	1.3	52
54	The nature of vertical excited states of dyes containing metals for DSSC applications: insights from TD-DFT and density based indexes. Physical Chemistry Chemical Physics, 2014, 16, 14435.	1.3	57

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55	Semiconductors Used in Photovoltaic and Photocatalytic Devices: Assessing Fundamental Properties from DFT. Journal of Physical Chemistry C, 2014, 118, 5997-6008.	1.5	239
56	Modeling Dye-Sensitized Solar Cells: From Theory to Experiment. Journal of Physical Chemistry Letters, 2013, 4, 1044-1050.	2.1	104
57	Through-Space Charge Transfer in Rod-Like Molecules: Lessons from Theory. Journal of Physical Chemistry C, 2012, 116, 11946-11955.	1.5	222
58	Promising anchoring groups for ZnOâ€based hybrid materials: A periodic density functional theory investigation. International Journal of Quantum Chemistry, 2012, 112, 2062-2071.	1.0	9
59	First-Principles Modeling of Dye-Sensitized Solar Cells: Challenges and Perspectives. Accounts of Chemical Research, 2012, 45, 1268-1277.	7.6	194
60	What is the â€œbestâ€•atomic charge model to describe through-space charge-transfer excitations?. Physical Chemistry Chemical Physics, 2012, 14, 5383.	1.3	290
61	Acetylacetone, an Interesting Anchoring Group for ZnO-Based Organicâ^'Inorganic Hybrid Materials: A Combined Experimental and Theoretical Study. Langmuir, 2011, 27, 3442-3450.	1.6	36
62	High Aspect Ratio Ternary Zn_{1â€“x}Cd_xO Nanowires by Electrodeposition for Light-Emitting Diode Applications. Journal of Physical Chemistry C, 2011, 115, 14548-14558.	1.5	69
63	A Qualitative Index of Spatial Extent in Charge-Transfer Excitations. Journal of Chemical Theory and Computation, 2011, 7, 2498-2506.	2.3	858
64	Theoretical Procedure for Optimizing Dye-Sensitized Solar Cells: From Electronic Structure to Photovoltaic Efficiency. Journal of the American Chemical Society, 2011, 133, 8005-8013.	6.6	85
65	Wavelengthâ€Emission Tuning of ZnO Nanowireâ€Based Lightâ€Emitting Diodes by Cu Doping: Experimental and Computational Insights. Advanced Functional Materials, 2011, 21, 3564-3572.	7.8	150
66	Acridine orange in a pumpkin-shaped macrocycle: Beyond solvent effects in the UVâ€“visible spectra simulation of dyes. Computational and Theoretical Chemistry, 2010, 954, 45-51.	1.5	10
67	Photophysical Properties of 8-Hydroxyquinoline-5-sulfonic Acid as a Function of the pH: A TD-DFT Investigation. Journal of Physical Chemistry A, 2010, 114, 5932-5939.	1.1	35
68	Effect of solvent and additives on the open-circuit voltage of ZnO-based dye-sensitized solar cells: a combined theoretical and experimental study. Physical Chemistry Chemical Physics, 2010, 12, 14710.	1.3	71
69	Electrodeposited Nanoporous versus Nanoparticulate ZnO Films of Similar Roughness for Dye-Sensitized Solar Cell Applications. ACS Applied Materials & Interfaces, 2010, 2, 3677-3685.	4.0	84
70	Theoretical determination of the pKas of the 8-hydroxyquinoline-5-sulfonic acid: A DFT based approach. Chemical Physics Letters, 2009, 472, 30-34.	1.2	36
71	A TD-DFT investigation of ground and excited state properties in indoline dyes used for dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2009, 11, 11276.	1.3	161