LluÃ-s Blancafort

List of Publications by Year
in descending order

107 papers	4,802 citations	100601 38 h-index	116156 66 g-index
114 all docs	114 docs citations	114 times ranked	4119 citing authors

#	Article	IF	Citations
1	Through-Space Interaction of Tetraphenylethylene: What, Where, and How. Journal of the American Chemical Society, 2022, 144, 7901-7910.	6.6	72
2	Switching between emission and photochemistry in an aggregationâ€induced emitter with extended conjugation. Aggregate, 2022, 3, .	5.2	1
3	Fingerprint-based deep neural networks can model thermodynamic and optical properties of eumelanin DHI dimers. Chemical Science, 2022, 13, 8942-8946.	3.7	1
4	Stability Studies of New Caged bis â€deoxyâ€coelenterazine Derivatives and Their Potential Use as Cellular pH Probes. Photochemistry and Photobiology, 2021, 97, 343-352.	1.3	0
5	Stability and Optical Absorption of a Comprehensive Virtual Library of Minimal Eumelanin Oligomer Models**. Angewandte Chemie - International Edition, 2021, 60, 18800-18809.	7.2	9
6	Stability and Optical Absorption of a Comprehensive Virtual Library of Minimal Eumelanin Oligomer Models**. Angewandte Chemie, 2021, 133, 18948-18957.	1.6	1
7	Rapid Activation of Diazirine Biomaterials with the Blue Light Photocatalyst. ACS Applied Materials & Interfaces, 2021, 13, 36839-36848.	4.0	10
8	Action spectroscopy of the isolated red Kaede fluorescent protein chromophore. Journal of Chemical Physics, 2021, 155, 124304.	1.2	9
9	Unusual Throughâ€Space Interactions between Oxygen Atoms that Mediate Inverse Morphochromism of an AIE Luminogen. Angewandte Chemie - International Edition, 2020, 59, 8552-8559.	7.2	28
10	Unusual Throughâ€Space Interactions between Oxygen Atoms that Mediate Inverse Morphochromism of an AIE Luminogen. Angewandte Chemie, 2020, 132, 8630-8637.	1.6	5
11	CaproGlu: Multifunctional tissue adhesive platform. Biomaterials, 2020, 260, 120215.	5.7	19
12	An nï€* gated decay mediates excited-state lifetimes of isolated azaindoles. Physical Chemistry Chemical Physics, 2020, 22, 18639-18645.	1.3	3
13	Locating Cytosine Conical Intersections by Laser Experiments and Ab Initio Calculations. Journal of Physical Chemistry Letters, 2020, 11, 3203-3210.	2.1	13
14	Computational Photochemistry. ChemPhotoChem, 2019, 3, 664-665.	1.5	1
15	Effects of Intra- and Intermolecular Hydrogen Bonding on Oâ€“H Bond Photodissociation Pathways of a Catechol Derivative. Journal of Physical Chemistry A, 2019, 123, 5356-5366.	1.1	14
16	Potentialâ€Energy Surface and Dynamics Simulation of THBDBA: An Annulated Tetraphenylethene Derivative Combining Aggregationâ€induced Emission and Switch Behavior. ChemPhotoChem, 2019, 3, 814-824.	1.5	12
17	Picosecond Switchable Azo Dyes. Chemistry - A European Journal, 2019, 25, 7726-7732.	1.7	25
18	Phosphorus-Doped Graphene as a Metal-Free Material for Thermochemical Water Reforming at Unusually Mild Conditions. ACS Sustainable Chemistry and Engineering, 2019, 7, 838-846.	3.2	28

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19	Exploring Potential Energy Surfaces for Aggregationâ€Induced Emissionâ€”From Solution to Crystal. Chemistry - an Asian Journal, 2019, 14, 700-714.	1.7	131
20	Intermolecular Hydrogen Bonding Modulates Oâ€H Photodissociation in Molecular Aggregates of a Catechol Derivative. Photochemistry and Photobiology, 2019, 95, 163-175.	1.3	19
21	Selfâ€Assembled Cofacial Zincâ€“Porphyrin Supramolecular Nanocapsules as Tuneable ¹O₂ Photosensitizers. Chemistry - A European Journal, 2018, 24, 4371-4381.	1.7	28
22	Thermally induced hopping model for long-range triplet excitation energy transfer in DNA. Physical Chemistry Chemical Physics, 2018, 20, 4997-5000.	1.3	10
23	A new twist in the photophysics of the GFP chromophore: a volume-conserving molecular torsion couple. Chemical Science, 2018, 9, 1803-1812.	3.7	36
24	Theoretical study of non-Hammett vs. Hammett behaviour in the thermolysis and photolysis of arylchlorodiazirines. Physical Chemistry Chemical Physics, 2018, 20, 1181-1188.	1.3	15
25	The Effect of Conjugation on the Competition between Internal Conversion and Electron Detachment: A Comparison between Green Fluorescent and Red Kaede Protein Chromophores. Journal of Physical Chemistry Letters, 2017, 8, 765-771.	2.1	17
26	Planarizing cytosine: The S1 state structure, vibrations, and nonradiative dynamics of jet-cooled 5,6-trimethylenecytosine. Journal of Chemical Physics, 2017, 146, 244308.	1.2	8
27	What Controls Photocatalytic Water Oxidation on Rutile TiO₂(110) under Ultra-High-Vacuum Conditions?. Journal of the American Chemical Society, 2017, 139, 11845-11856.	6.6	48
28	Direct estimation of the transfer integral for photoinduced electron transfer from TD DFT calculations. Physical Chemistry Chemical Physics, 2017, 19, 31007-31010.	1.3	3
29	The excited-state structure, vibrations, lifetimes, and nonradiative dynamics of jet-cooled 1-methylcytosine. Journal of Chemical Physics, 2016, 145, 134307.	1.2	16
30	Synthesis and Isomeric Analysis of Ru^{II} Complexes Bearing Pentadentate Scaffolds. Inorganic Chemistry, 2016, 55, 11216-11229.	1.9	17
31	Excitonic Interfacial Proton-Coupled Electron Transfer Mechanism in the Photocatalytic Oxidation of Methanol to Formaldehyde on TiO₂(110). Journal of the American Chemical Society, 2016, 138, 16165-16173.	6.6	64
32	Early events in the photochemistry of 5-diazo Meldrum's acid: formation of a product manifold in Câ€“N bound and pre-dissociated intersection seam regions. Physical Chemistry Chemical Physics, 2016, 18, 30785-30793.	1.3	11
33	Multiple Decay Mechanisms and 2Dâ€UV Spectroscopic Fingerprints of Singlet Excited Solvated Adenineâ€Uracil Monophosphate. Chemistry - A European Journal, 2016, 22, 7497-7507.	1.7	31
34	Triplet Mediated Câ€“N Dissociation versus Internal Conversion in Electronically Excited N-Methylpyrrole. Journal of Physical Chemistry Letters, 2016, 7, 1231-1237.	2.1	14
35	Quantum Mechanical Studies on the Photophysics and the Photochemistry of Nucleic Acids and Nucleobases. Chemical Reviews, 2016, 116, 3540-3593.	23.0	375
36	Restricted access to a conical intersection to explain aggregation induced emission in dimethyl tetraphenylsilole. Journal of Materials Chemistry C, 2016, 4, 2802-2810.	2.7	144

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37	Disaggregation-induced fluorescence enhancement of NIAD-4 for the optical imaging of amyloid-Î² fibrils. Physical Chemistry Chemical Physics, 2015, 17, 19718-19725.	1.3	24
38	Conical Intersection Optimization Using Composed Steps Inside the ONIOM(QM:MM) Scheme: CASSCF:UFF Implementation with Microiterations. Journal of Chemical Theory and Computation, 2015, 11, 1585-1594.	2.3	33
39	Polarizable QM/MM Multiconfiguration Self-Consistent Field Approach with State-Specific Corrections: Environment Effects on Cytosine Absorption Spectrum. Journal of Chemical Theory and Computation, 2015, 11, 1674-1682.	2.3	43
40	Exciton delocalization, charge transfer, and electronic coupling for singlet excitation energy transfer between stacked nucleobases in DNA: An MS-CASPT2 study. Journal of Chemical Physics, 2014, 140, 095102.	1.2	46
41	Photochemistry and Photophysics at Extended Seams of Conical Intersection. ChemPhysChem, 2014, 15, 3166-3181.	1.0	74
42	On the performance of the Kohnâ€“Sham orbital approach in the calculation of electron transfer parameters. The three state model. Physical Chemistry Chemical Physics, 2014, 16, 17154-17162.	1.3	4
43	The response of the electronic structure to electronic excitation and double bond torsion in fulvene: a combined QTAIM, stress tensor and MO perspective. Physical Chemistry Chemical Physics, 2014, 16, 7115-7126.	1.3	58
44	Photophysics of fulvene under the non-resonant stark effect. Shaping the conical intersection seam. Faraday Discussions, 2013, 163, 497.	1.6	17
45	Photochemistry and photophysics of the amino and imino tautomers of 1-methylcytosine: tautomerisation as a side product of the radiationless decay. Photochemical and Photobiological Sciences, 2013, 12, 1401-1408.	1.6	22
46	A conical intersection model to explain aggregation induced emission in diphenyl dibenzofulvene. Chemical Communications, 2013, 49, 5966.	2.2	158
47	Ultrafast above-threshold dynamics of the radical anion of a prototypical quinone electron-acceptor. Nature Chemistry, 2013, 5, 711-717.	6.6	76
48	Conical Intersection Optimization Based on a Double Newtonâ€“Raphson Algorithm Using Composed Steps. Journal of Chemical Theory and Computation, 2013, 9, 1433-1442.	2.3	21
49	A Valence Bond Description of the Prefulvene Extended Conical Intersection Seam of Benzene. Journal of Chemical Theory and Computation, 2012, 8, 4922-4930.	2.3	29
50	Irreversible phototautomerization of o-phthalaldehyde through electronic relocation. Physical Chemistry Chemical Physics, 2012, 14, 6561.	1.3	19
51	Wave Packet Dynamics at an Extended Seam of Conical Intersection: Mechanism of the Light-Induced Wolff Rearrangement. Journal of Physical Chemistry Letters, 2012, 3, 1056-1061.	2.1	32
52	MS-CASPT2 Study of Hole Transfer in Guanineâ€“Indole Complexes Using the Generalized Mullikenâ€“Hush Method: Effective Two-State Treatment. Journal of Physical Chemistry B, 2012, 116, 7815-7820.	1.2	4
53	Role of Hyperconjugation in the 1,2-Shift Reactivity of Bicyclo[2.1.0]pentane and Cyclopropane Radical Cations: A Computational Study. Journal of Physical Chemistry A, 2012, 116, 10607-10614.	1.1	6
54	Ultrafast irreversible phototautomerization of o-nitrobenzaldehyde. Chemical Communications, 2011, 47, 6383.	2.2	33

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55	Local Excitation of the 5-Bromouracil Chromophore in DNA. Computational and UV Spectroscopic Studies. Journal of Physical Chemistry B, 2011, 115, 4532-4537.	1.2	8
56	A non-adiabatic quantum-classical dynamics study of the intramolecular excited state hydrogen transfer in ortho-nitrobenzaldehyde. Physical Chemistry Chemical Physics, 2011, 13, 14685.	1.3	17
57	Quantum dynamics study of fulvene double bond photoisomerization: The role of intramolecular vibrational energy redistribution and excitation energy. Journal of Chemical Physics, 2011, 135, 134303.	1.2	24
58	A global picture of the S1/S0 conical intersection seam of benzene. Chemical Physics, 2010, 377, 60-65.	0.9	61
59	Exploring the sloped-to-peaked S2/S1 seam of intersection of thymine with electronic structure and direct quantum dynamics calculations. Physical Chemistry Chemical Physics, 2010, 12, 4949.	1.3	83
60	Tuning aromaticity in trigonal alkaline earth metal clusters and their alkali metal salts. Journal of Computational Chemistry, 2009, 30, 2764-2776.	1.5	43
61	Excess charge delocalization in organic and biological molecules: some theoretical notions. Theoretical Chemistry Accounts, 2009, 123, 29-40.	0.5	9
62	MS-CASPT2 Assignment of the UV/Vis Absorption Spectrum of Diazoquinones Undergoing the Photoinduced Wolff Rearrangement. Journal of Physical Chemistry A, 2009, 113, 9413-9417.	1.1	13
63	Benign Decay vs. Photolysis in the Photophysics and Photochemistry of 5-Bromouracil. A Computational Study. Journal of Physical Chemistry A, 2009, 113, 5489-5495.	1.1	19
64	Photophysics of the Ï€,Ï€* and n,Ï€* States of Thymine: MS-CASPT2 Minimum-Energy Paths and CASSCF on-the-Fly Dynamics. Journal of Physical Chemistry A, 2009, 113, 10211-10218.	1.1	83
65	Second-Order Analysis of Conical Intersections: Applications to Photochemistry and Photophysics of Organic Molecules. Springer Series in Chemical Physics, 2009, , 169-200.	0.2	7
66	New Algorithms for Optimizing and Linking Conical Intersection Points. Journal of Chemical Theory and Computation, 2008, 4, 257-266.	2.3	97
67	Electronic States of o-Nitrobenzaldehyde: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 5046-5053.	1.1	30
68	An Extended Conical Intersection Seam Associated with a Manifold of Decay Paths: Excited-State Intramolecular Proton Transfer in O-Hydroxybenzaldehyde. Journal of the American Chemical Society, 2008, 130, 6932-6933.	6.6	64
69	Automatic generation of active coordinates for quantum dynamics calculations: Application to the dynamics of benzene photochemistry. Journal of Chemical Physics, 2008, 128, 124307.	1.2	39
70	Chapter 3 The breakdown of the maximum hardness and minimum polarizability principles for nontotally symmetric vibrations. Theoretical and Computational Chemistry, 2007, , 31-45.	0.2	2
71	Modeling Thymine Photodimerizations in DNA:â€‰ Mechanism and Correlation Diagrams. Journal of the American Chemical Society, 2007, 129, 14540-14541.	6.6	88
72	Quadratic Description of Conical Intersections:â€‰ Characterization of Critical Points on the Extended Seam. Journal of Physical Chemistry A, 2007, 111, 2182-2192.	1.1	70

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73	MS-CASPT2 Calculation of Excess Electron Transfer in Stacked DNA Nucleobases. Journal of Physical Chemistry A, 2007, 111, 4714-4719.	1.1	28
74	Benign and Degrading Excited-State Processes of DNA Nucleobases and their Derivatives. AIP Conference Proceedings, 2007, , .	0.3	0
75	Water effect on the excited-state decay paths of singlet excited cytosine. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 283-289.	2.0	43
76	Energetics of Cytosine Singlet Excited-State Decay Paths-A Difficult Case for CASSCF and CASPT2â€. Photochemistry and Photobiology, 2007, 83, 603-610.	1.3	79
77	An analytical second-order description of the S 0 /S 1 intersection seam: fulvene revisited. Theoretical Chemistry Accounts, 2007, 118, 241-251.	0.5	53
78	Canonical Watsonâ€“Crick base pair interactions in Ï€â€‰â†'â€‰Ï€* type triplet states. Molecular Physics, 2006, 104, 925-931.	0.8	5
79	Pseudo-Jahnâ^'Teller Effect as the Origin of the Exalted Frequency of the b2u KekulÃ© Mode in the 1B2u Excited State of Benzene. Journal of Physical Chemistry A, 2006, 110, 11219-11222.	1.1	23
80	Mapping the intersection space of the ground and first excited states of fulvene. Molecular Physics, 2006, 104, 1033-1038.	0.8	27
81	Excited-State Potential Energy Surface for the Photophysics of Adenine. Journal of the American Chemical Society, 2006, 128, 210-219.	6.6	158
82	CASSCF/CAS-PT2 Study of Hole Transfer in Stacked DNA Nucleobases. Journal of Physical Chemistry A, 2006, 110, 6426-6432.	1.1	94
83	Ring puckering of cyclooctatetraene and cyclohexane is induced by pseudo-Jahnâ€“Teller coupling. Molecular Physics, 2006, 104, 2007-2010.	0.8	29
84	Conical intersections: A perspective on the computation of spectroscopic Jahnâ€“Teller parameters and the degenerate â€˜intersection spaceâ€™. Physical Chemistry Chemical Physics, 2005, 7, 2100.	1.3	67
85	Intramolecular Electron Transfer in Bis(methylene) Adamantyl Radical Cation:Â A Case Study of Diabatic Trapping. Journal of the American Chemical Society, 2005, 127, 3391-3399.	6.6	46
86	Mechanism of an Exceptional Class of Photostabilizers:Â A Seam of Conical Intersection Parallel to Excited State Intramolecular Proton Transfer (ESIPT) ino-Hydroxyphenyl-(1,3,5)-triazine. Journal of Physical Chemistry A, 2005, 109, 7527-7537.	1.1	111
87	Singlet Excited-State Dynamics of 5-Fluorocytosine and Cytosine:Â An Experimental and Computational Study. Journal of Physical Chemistry A, 2005, 109, 4431-4436.	1.1	104
88	Triplet-State Formation along the Ultrafast Decay of Excited Singlet Cytosine. Journal of the American Chemical Society, 2005, 127, 1820-1825.	6.6	175
89	Triplet (Ï€,Ï€*) Reactivity of the Guanineâ^'Cytosine DNA Base Pair:Â Benign Deactivation versus Double Tautomerization via Intermolecular Hydrogen Transfer. Journal of the American Chemical Society, 2004, 126, 12770-12771.	6.6	23
90	Key Role of a Threefold State Crossing in the Ultrafast Decay of Electronically Excited Cytosine. Journal of Physical Chemistry A, 2004, 108, 10609-10614.	1.1	122

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91	Theoretical Study of Benzotriazole UV Photostability:Â Ultrafast Deactivation through Coupled Proton and Electron Transfer Triggered by a Charge-Transfer State. Journal of the American Chemical Society, 2004, 126, 2912-2922.	6.6	132
92	The curvature of the conical intersection seam: An approximate second-order analysis. Journal of Chemical Physics, 2004, 121, 11562-11571.	1.2	57
93	A valence-bond-based complete-active-space self-consistent-field method for the evaluation of bonding in organic molecules. Theoretical Chemistry Accounts, 2003, 110, 92-99.	0.5	38
94	Evaluation of the Analogy between Exceptions to the Generalized Maximum Hardness Principle for Non-Totally-Symmetric Vibrations and the Pseudo-Jahnâ˜Teller Effect. Journal of Physical Chemistry A, 2003, 107, 7337-7339.	1.1	18
95	A new efficient approach to the direct restricted active space self-consistent field method. Journal of Chemical Physics, 2003, 119, 713-728.	1.2	28
96	Quenching of Tryptophan 1(Ï€,Ï€*) Fluorescence Induced by Intramolecular Hydrogen Abstraction via an Aborted Decarboxylation Mechanism. Journal of the American Chemical Society, 2002, 124, 6398-6406.	6.6	43
97	Photoinduced Electron Transfer in Squaraine Dyes:â€‰ Sensitization of Large Band Gap Semiconductors. Journal of Physical Chemistry A, 2002, 106, 11431-11439.	1.1	29
98	The pseudo-Jahnâ€”Teller effect: a CASSCF diagnostic. Molecular Physics, 2002, 100, 1735-1739.	0.8	43
99	Ultrafast Decay of Electronically Excited Singlet Cytosine via a Ï€,Ï€* to nO,Ï€* State Switch. Journal of the American Chemical Society, 2002, 124, 6818-6819.	6.6	302
100	Potential Energy Surface Crossings and the Mechanistic Spectrum for Intramolecular Electron Transfer in Organic Radical Cations. Journal of the American Chemical Society, 2001, 123, 722-732.	6.6	67
101	The Valence Isomerization of Cyclooctatetraene to Semibullvalene. Angewandte Chemie - International Edition, 2000, 39, 2095-2097.	7.2	25
102	Intramolecular Electron Transfer:â€‰ Independent (Ground State) Adiabatic (Chemical) and Nonadiabatic Reaction Pathways in Bis(hydrazine) Radical Cations. Journal of the American Chemical Society, 2000, 122, 7528-7533.	6.6	37
103	Theoretical Study of the 1,2 Rearrangement of Housane Radical Cations:Â Key Role of a Transient Cyclopentane-1,3-diyl Intermediate. Journal of the American Chemical Society, 1999, 121, 10583-10590.	6.6	24
104	Reaction of Î±-Peroxy Lactones with C, N, P, and S Nucleophiles:Â Adduct Formation and Nucleophile Oxidation by Nucleophilic Attack at and Biphilic Insertion into the Peroxide Bond. Journal of Organic Chemistry, 1997, 62, 1623-1629.	1.7	23
105	Kinetic resolution of racemic halohydrins, precursors of optically active di- and trialkyl-substituted epoxides, with lipase from Pseudomonas sp.. Tetrahedron: Asymmetry, 1997, 8, 3189-3192.	1.8	12
106	Stereoselective Cycloaddition and Epoxidation of Enol Ethers by Î±-Peroxy Lactone as a Function of Steric and Stereoelectronic Effects. Journal of Organic Chemistry, 1996, 61, 8432-8438.	1.7	11
107	Steric and Stereoelectronic Control of the Mode Selectivity as a Function of Alkene Structure in the Reaction with Dimethyl Î±-Peroxy Lactone:Â Cycloadducts and Ene ProductsversusEpoxides. Journal of the American Chemical Society, 1996, 118, 4778-4787.	6.6	20