christophe Morell

List of Publications by Year
in descending order

81 papers	3,479 citations	218381 26 h-index	143772 57 g-index
87 all docs	87 docs citations	87 times ranked	2353 citing authors

#	Article	IF	Citations
1	Reactivity and a Charge-Transfer Model Analysis in Aminopolycarboxylicâ€“Metal Complexes. Inorganic Chemistry, 2022, 61, 4673-4680.	1.9	0
2	A computational investigation of the selectivity and mechanism of the Lewis acid catalyzed oxaâ€Dielsâ€“Alder cycloaddition of substituted diene with benzaldehyde. Journal of Computational Chemistry, 2021, 42, 1296-1311.	1.5	10
3	The density polarization reveals directions of electron displacements due to the substituent effect: Analysis performed on a metalâ€organic Moâ€Oxo catalyst. Journal of Computational Chemistry, 2021, 42, 1118-1125.	1.5	0
4	Understanding the intermolecular Dielsâ€“Alder cycloaddition promotion: Activation strain model/energy decomposition analysis model and conceptual density functional theory viewpoints. Journal of Computational Chemistry, 2021, 42, 1364-1372.	1.5	3
5	A Dynamic View of the Interaction of Histone Tails with Clustered Abasic Sites in a Nucleosome Core Particle. Journal of Physical Chemistry Letters, 2021, 12, 6014-6019.	2.1	10
6	Predicted structure and selectivity of 3d transition metal complexes with glutamicN,N-bis(carboxymethyl) acid. New Journal of Chemistry, 2021, 45, 18366-18378.	1.4	5
7	Polarisation of Electron Density and Electronic Effects: Revisiting the Carbonâ€“Halogen Bonds. Molecules, 2021, 26, 6218.	1.7	2
8	Understanding Chemical Selectivity through Well Selected Excited States. Journal of Physical Chemistry A, 2020, 124, 633-641.	1.1	16
9	Relaxation of Kohnâ€“Sham orbitals of organometallic complexes during the approach of a nucleophilic reactant (or an electron approach): the case of [sal(ph)en]2 Zn complexes. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	3
10	A statistical thermodynamics view of electron density polarisation: application to chemical selectivity. Physical Chemistry Chemical Physics, 2020, 22, 23553-23562.	1.3	7
11	Nucleosomal embedding reshapes the dynamics of abasic sites. Scientific Reports, 2020, 10, 17314.	1.6	13
12	Conceptual density functional theory: status, prospects, issues. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	249
13	Coordination chemistry of Zn²⁺ with Sal(ph)en ligands: Tetrahedral coordination or pentaâ€coordination? a DFT analysis. Journal of Computational Chemistry, 2019, 40, 717-725.	1.5	15
14	Substituent Effect on the Himbert Intramolecular Arene/Allene Dielsâ€“Alder Reaction: NBO Analysis and State Specific Dual Descriptors. Journal of Physical Chemistry A, 2019, 123, 10730-10738.	1.1	7
15	Evidencing under-barrier phenomena in a Yb(<scp>iii</scp>) SMM: a joint luminescence/neutron diffraction/SQUID study. Inorganic Chemistry Frontiers, 2019, 6, 3152-3157.	3.0	24
16	Wetting the lock and key enthalpically favours polyelectrolyte binding. Chemical Science, 2019, 10, 277-283.	3.7	8
17	Theoretical study of the mechanism and regioselectivity in the formation of pyrazolo[1,5-a]-[1,3,5]-triazines and pyrazolo[1,5-a]-[1,3,5]triazinones: A DFT study. Chemical Physics Letters, 2019, 727, 95-104.	1.2	8
18	Does the gradientâ€regulated connection improve the description of correlated metal bond properties?. International Journal of Quantum Chemistry, 2019, 119, e25831.	1.0	0

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19	Raman spectroscopy combined with advanced chemometric methods: A new approach for detergent deformulation. Talanta, 2019, 195, 441-446.	2.9	7
20	Comment on â€œRevisiting the definition of local hardness and hardness kernelâ€• by C. A. Polanco-Ramirez, M. Franco-PÃ©rez, J. Carmona-EspÃndola, J. L. GÃ¡zquez and P. W. Ayers, Phys. Chem. Chem. Phys., 2017, 19, 12355. Physical Chemistry Chemical Physics, 2018, 20, 9006-9010.	1.3	7
21	Teaching an old molecule new tricks: evidence and rationalisation of the slow magnetisation dynamics in [DyTp₂Acac]. Inorganic Chemistry Frontiers, 2018, 5, 1346-1353.	3.0	15
22	Unexpected Structure of a Helical N₄â€“Schiffâ€“Base Zn(II) Complex and Its Demetallation: Experimental and Theoretical Studies. ChemPhysChem, 2018, 19, 2938-2946.	1.0	10
23	Combined QTAIM and ETS-NOCV investigation of the interactions in ClnM[PhB(NtBu)2] complexes with Mâ€‰=â€‰Si & Ge (nâ€‰=â€‰0), As & Sb (nâ€‰=â€‰1), Te & Po (nâ€‰=â€‰2). Journal of Molecular Modeling, 2018, 24, 327.	0.8	0
24	Fluorine substituent effect on the stereochemistry of catalyzed and non-catalyzed Dielsâ€“Alder reactions. The case of R-butenone with cyclopentadiene: a computational assessment of the mechanism. Physical Chemistry Chemical Physics, 2018, 20, 16102-16116.	1.3	12
25	Interstrand cross-linking implies contrasting structural consequences for DNA: insights from molecular dynamics. Nucleic Acids Research, 2017, 45, gkw1253.	6.5	10
26	Conformational polymorphism or structural invariance in DNA photoinduced lesions: implications for repair rates. Nucleic Acids Research, 2017, 45, 3654-3662.	6.5	17
27	Ibuprofen and ketoprofen potentiate UVA-induced cell death by a photosensitization process. Scientific Reports, 2017, 7, 8885.	1.6	19
28	Molecular Dynamics Insights into Polyamineâ€“DNA Binding Modes: Implications for Crossâ€Link Selectivity. Chemistry - A European Journal, 2017, 23, 12845-12852.	1.7	34
29	Conceptual DFT analysis of the regioselectivity of 1,3-dipolar cycloadditions: nitrones as a case of study. Journal of Molecular Modeling, 2017, 23, 236.	0.8	15
30	Structural effects in octahedral carbonyl complexes: an atoms-in-molecules study. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	8
31	Repair Rate of Clustered Abasic DNA Lesions by Human Endonuclease: Molecular Bases of Sequence Specificity. Journal of Physical Chemistry Letters, 2016, 7, 3760-3765.	2.1	30
32	Correlation of bistranded clustered abasic DNA lesion processing with structural and dynamic DNA helix distortion. Nucleic Acids Research, 2016, 44, 8588-8599.	6.5	37
33	Singlet Oxygen Attack on Guanine: Reactivity and Structural Signature within the Bâ€DNA Helix. Chemistry - A European Journal, 2016, 22, 12358-12362.	1.7	34
34	Acute aquatic toxicity of organic solvents modeled by QSARs. Journal of Molecular Modeling, 2016, 22, 288.	0.8	30
35	Solvent database and in silico classification: A new methodology for solvent substitution and its application for microencapsulation process. International Journal of Pharmaceutics, 2016, 509, 454-464.	2.6	6
36	Ill-advised self-interaction contribution in modelling anionic attack along a reaction path. Molecular Physics, 2016, 114, 1066-1075.	0.8	3

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37	Probing the reactivity of singlet oxygen with purines. Nucleic Acids Research, 2016, 44, 56-62.	6.5	57
38	Towards the first theoretical scale of the trans effect in octahedral complexes. Physical Chemistry Chemical Physics, 2016, 18, 982-990.	1.3	24
39	DNA Photosensitization by an â€œInsiderâ€• Photophysics and Triplet Energy Transfer of 5â€Methylâ€2â€pyrimidone Deoxyribonucleoside. Chemistry - A European Journal, 2015, 21, 11509-11516.	1.7	19
40	Proton Migration in Clusters Consisting of Protonated Pyridine Solvated by Water Molecules. ChemPhysChem, 2015, 16, 3151-3155.	1.0	11
41	Quantifying electro/nucleophilicity by partitioning the dual descriptor. Journal of Computational Chemistry, 2015, 36, 649-659.	1.5	39
42	Investigation of electron density changes at the onset of a chemical reaction using the state-specific dual descriptor from conceptual density functional theory. Physical Chemistry Chemical Physics, 2015, 17, 9359-9368.	1.3	29
43	Atomic electronegativities in molecules. Chemical Physics Letters, 2015, 635, 111-115.	1.2	19
44	Allylation of active methylene compounds with cyclic Baylisâ€“Hillman alcohols: a DFT study. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	4
45	Insights into the chemical meanings of the reaction electronic flux. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	20
46	Characterization of the Chemical Reactivity and Selectivity of DNA Bases Through the Use of DFT-Based Descriptors. Topics in Heterocyclic Chemistry, 2014, , 35-70.	0.2	3
47	Electron Paramagnetic Resonance Tracing of Electronic Transfers in Pushâ€“Pull Copolymers/PCBM or Nanocrystal Composites. Journal of Physical Chemistry C, 2014, 118, 20647-20660.	1.5	6
48	Revisiting electroaccepting and electrodonating powers: proposals for local electrophilicity and local nucleophilicity descriptors. Physical Chemistry Chemical Physics, 2014, 16, 26832-26842.	1.3	68
49	Dual descriptor and molecular electrostatic potential: complementary tools for the study of the coordination chemistry of ambiphilic ligands. Physical Chemistry Chemical Physics, 2014, 16, 15558-15569.	1.3	36
50	Deamination features of 5-hydroxymethylcytosine, a radical and enzymatic DNA oxidation product. Journal of Molecular Modeling, 2014, 20, 2290.	0.8	3
51	DFT study of the stereo-selectivity of oxygenated heterocycles from 10 to 12 links. Canadian Journal of Chemistry, 2013, 91, 811-820.	0.6	0
52	A proposal for an extended dual descriptor: a possible solution when Frontier Molecular Orbital Theory fails. Physical Chemistry Chemical Physics, 2013, 15, 14465.	1.3	67
53	Is hyper-hardness more chemically relevant than expected?. Journal of Molecular Modeling, 2013, 19, 2893-2900.	0.8	60
54	UV-induced formation of the thymine-thymine pyrimidine (6-4) pyrimidone photoproduct â€” a DFT study of the oxetane intermediate ring opening. Photochemical and Photobiological Sciences, 2013, 12, 1509-1516.	1.6	13

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55	Comparison of the mechanism of deamination of 5,6-dihydro-5-methylcytosine with other cytosine derivatives. Highlights in Theoretical Chemistry, 2013, , 307-317.	0.0	0
56	A Relation between Different Scales of Electrophilicity: Are the Scales Consistent Along a Chemical Reaction?. Journal of Physical Chemistry A, 2012, 116, 7074-7081.	1.1	9
57	Comparison of the mechanism of deamination of 5,6-dihydro-5-methylcytosine with other cytosine derivatives. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	5
58	Use of the Dual Potential to Rationalize the Occurrence of Some DNA Lesions (Pyrimidic Dimers). Journal of Physical Chemistry A, 2011, 115, 8032-8040.	1.1	11
59	Application of the electron density force to chemical reactivity. Physical Chemistry Chemical Physics, 2011, 13, 9601.	1.3	15
60	New Alternating Copolymers of 3,6â€Carbazoles and Dithienylbenzothiadiazoles: Synthesis, Characterization, and Application in Photovoltaics. Macromolecular Chemistry and Physics, 2011, 212, 2127-2141.	1.1	21
61	Extending the â€˜Grochalaâ€“Albrechtâ€“Hoffmann approximationâ€™ to the determination of the first excited state potential energy profile of a reaction step. Chemical Physics Letters, 2010, 485, 371-375.	1.2	8
62	Hydrolytic Deamination of 5,6-Dihydrocytosine in a Protic Medium: A Theoretical Study. Journal of Physical Chemistry A, 2010, 114, 1826-1834.	1.1	24
63	Is an elementary reaction step really elementary? Theoretical decomposition of asynchronous concerted mechanisms. Physical Chemistry Chemical Physics, 2010, 12, 4142.	1.3	30
64	Characterization of the Chemical Behavior of the Low Excited States through a Local Chemical Potential. Journal of Chemical Theory and Computation, 2009, 5, 2274-2283.	2.3	31
65	Minimum electrophilicity principle: an analysis based upon the variation of both chemical potential and absolute hardness. Physical Chemistry Chemical Physics, 2009, 11, 3417.	1.3	71
66	Chemical Reactivity Descriptors for Ambiphilic Reagents: Dual Descriptor, Local Hypersoftness, and Electrostatic Potential. Journal of Physical Chemistry A, 2009, 113, 8660-8667.	1.1	166
67	Hydrolytic Deamination of 5-Methylcytosine in Protic Mediumâ€”A Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 2524-2533.	1.1	45
68	Mechanism of nitric oxide induced deamination of cytosine. Physical Chemistry Chemical Physics, 2009, 11, 2379.	1.3	10
69	Proton catalyzed hydrolytic deamination of cytosine: a computational study. Theoretical Chemistry Accounts, 2008, 120, 429-435.	0.5	28
70	A conceptual DFT study of hydrazino peptides: Assessment of the nucleophilicity of the nitrogen atoms by means of the dual descriptor Î”f(r). Computational and Theoretical Chemistry, 2008, 849, 46-51.	1.5	54
71	Rationalization of Dielsâ€“Alder reactions through the use of the dual reactivity descriptor Î”f(r). Physical Chemistry Chemical Physics, 2008, 10, 7239.	1.3	94
72	Theoretical Study of Cytosine Deamination from the Perspective of the Reaction Force Analysis. Journal of Physical Chemistry A, 2008, 112, 11487-11494.	1.1	38

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73	Formation of cross-linked adducts between guanine and thymine mediated by hydroxyl radical and one-electron oxidation: a theoretical study. Organic and Biomolecular Chemistry, 2008, 6, 3300.	1.5	53
74	Chapter 7 Using the reactivity-selectivity descriptor Î” f(r) in organic chemistry. Theoretical and Computational Chemistry, 2007, , 101-117.	0.2	8
75	â€¢H Atom andâ€¢OH Radical Reactions with 5-Methylcytosine. Journal of Physical Chemistry A, 2007, 111, 8968-8972.	1.1	23
76	Understanding the Woodwardâ€“Hoffmann Rules by Using Changes in Electron Density. Chemistry - A European Journal, 2007, 13, 8240-8247.	1.7	216
77	Radiation-induced formation of DNA intrastrand crosslinks between thymine and adenine bases: a theoretical approach. Organic and Biomolecular Chemistry, 2006, 4, 3986.	1.5	29
78	Theoretical support for using the Î”f(r) descriptor. Chemical Physics Letters, 2006, 425, 342-346.	1.2	320
79	New Dual Descriptor for Chemical Reactivity. Journal of Physical Chemistry A, 2005, 109, 205-212.	1.1	978
80	Theoretical Study of the Internal Rotation of the Hydroxylic Group of the Enol Form of Guanine. Journal of Physical Chemistry A, 2003, 107, 5334-5341.	1.1	33
81	Molecular Interactions From the Density Functional Theory for Chemical Reactivity: The Interaction Energy Between Two-Reagents. Frontiers in Chemistry, 0, 10, .	1.8	6