Bernard Silvi

List of Publications by Year
in descending order

79 papers	6,553 citations	81900 39 h-index	74163 75 g-index
80 all docs	80 docs citations	80 times ranked	3586 citing authors

#	Article	IF	Citations
1	Towards an unified chemical model of secondary bonding. Journal of Molecular Modeling, 2020, 26, 62.	1.8	14
2	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	3.3	113
3	The Mysticism of Pericyclic Reactions: A Contemporary Rationalisation of Organic Reactivity Based on Electron Density Analysis. European Journal of Organic Chemistry, 2018, 2018, 1107-1120.	2.4	69
4	Pressure effect on electron localization in solid lithium. Structural Chemistry, 2017, 28, 1389-1397.	2.0	9
5	Topological analysis of the metal-metal bond: A tutorial review. Coordination Chemistry Reviews, 2017, 345, 150-181.	18.8	108
6	Curly arrows, electron flow, and reaction mechanisms from the perspective of the bonding evolution theory. Physical Chemistry Chemical Physics, 2017, 19, 29031-29046.	2.8	36
7	About Lewisâ€™s heritage: chemical interpretations and quantum chemistry. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	6
8	Curly arrows meet electron density transfers in chemical reaction mechanisms: from electron localization function (ELF) analysis to valence-shell electron-pair repulsion (VSEPR) inspired interpretation. Chemical Communications, 2016, 52, 8183-8195.	4.1	66
9	Topological Approaches of the Bonding in Conceptual Chemistry. Challenges and Advances in Computational Chemistry and Physics, 2016, , 1-20.	0.6	3
10	Hydrogen bonding and delocalization in the ELF analysis approach. Physical Chemistry Chemical Physics, 2016, 18, 27442-27449.	2.8	27
11	Activation of Câ€“H and Bâ€“H bonds through agostic bonding: an ELF/QTAIM insight. Physical Chemistry Chemical Physics, 2015, 17, 9258-9281.	2.8	36
12	The Missing Entry in the Agosticâ€“Anagostic Series: Rh(I)â€“Î·¹-C Interactions in P(CH)P Pincer Complexes. Inorganic Chemistry, 2015, 54, 2960-2969.	4.0	46
13	The Relevance of the ELF Topological Approach to the Lewis, Kossel, and Langmuir Bond Model. Structure and Bonding, 2015, , 213-247.	1.0	6
14	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	2.5	99
15	Atoms and bonds in molecules and chemical explanations. Foundations of Chemistry, 2014, 16, 3-26.	1.1	17
16	Carbolithiation of Chloroâ€Substituted Alkynes: A New Access to Vinyl Carbenoids. Chemistry - A European Journal, 2014, 20, 10249-10254.	3.3	22
17	Coupling Quantum Interpretative Techniques: Another Look at Chemical Mechanisms in Organic Reactions. Journal of Chemical Theory and Computation, 2012, 8, 3993-3997.	5.3	104
18	Electronic fluxes during dielsâ€alder reactions involving 1,2â€benzoquinones: mechanistic insights from the analysis of electron localization function and catastrophe theory. Journal of Computational Chemistry, 2012, 33, 2400-2411.	3.3	26

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19	Bonding Changes Along Solid-Solid Phase Transitions Using the Electron Localization Function Approach. , 2011, , 625-658.		3
20	Localization and Localizability in Quantum Organic Chemistry: Localized Orbitals and Localization Functions. Current Organic Chemistry, 2011, 15, 3555-3565.	1.6	5
21	N, P, and As Ylides and Aza- and Arsa-Wittig Reactions from Topological Analyses of Electron Density. Journal of Physical Chemistry A, 2011, 115, 8316-8326.	2.5	12
22	XeF₂Coordination to a Halogen Center; Raman Spectra (n= 1, 2) and X-ray Crystal Structures (n= 2) of [BrOF₂][AsF₆]Â·nXeF₂and [XOF₂][AsF₆] (X = Cl, Br). Inorganic Chemistry, 2010, 49, 6673-6689.	4.0	29
23	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2010, 6, 2736-2742.	5.3	115
24	Is delocalization a prerequisite for stability of ring systems? A case study of some inorganic rings. Dalton Transactions, 2010, 39, 4126.	3.3	33
25	A Rare Example of a Krypton Difluoride Coordination Compound: [BrOF₂][AsF₆]Â·2KrF₂. Journal of the American Chemical Society, 2010, 132, 3533-3542.	13.7	37
26	Understanding Reaction Mechanisms in Organic Chemistry from Catastrophe Theory: Ozone Addition on Benzene. Journal of Physical Chemistry A, 2010, 114, 12900-12906.	2.5	19
27	Topological Analysis of the Interactions between Organic Molecules and Co(Ni)MoS Catalytic Active Phases. Journal of Chemical Theory and Computation, 2009, 5, 580-593.	5.3	11
28	Useful applications of the electron localization function in high-pressure crystal chemistry. Journal of Physics and Chemistry of Solids, 2008, 69, 2204-2207.	4.0	25
29	An electron localization function and catastrophe theory analysis on the molecular mechanism of gas-phase identity SN2 reactions. Theoretical Chemistry Accounts, 2008, 120, 341-349.	1.4	41
30	Understanding Reaction Mechanisms in Organic Chemistry from Catastrophe Theory Applied to the Electron Localization Function Topology. Journal of Physical Chemistry A, 2008, 112, 7128-7136.	2.5	165
31	On the Bonding of Selenocyanates and Isoselenocyanates and Their Protonated Derivatives. Journal of Chemical Theory and Computation, 2008, 4, 1593-1599.	5.3	8
32	Quantifying the Donorâ"Acceptor Properties of Carbon Monoxide and ItsCarbo-mer Using ELF Analysis. Organometallics, 2008, 27, 5263-5272.	2.3	13
33	Topological Analysis of the Reaction of Uranium Ions (U⁺, U²⁺) with N₂O in the Gas Phase. Journal of Physical Chemistry A, 2008, 112, 12966-12974.	2.5	45
34	Chapter 4 Classification of control space parameters for topological studies of reactivity and chemical reactions. Theoretical and Computational Chemistry, 2007, 19, 47-56.	0.4	1
35	Combined Theoretical and Experimental Analysis of the Bonding in the Heterobimetallic Cubane-Type Mo3NiS4and Mo3CuS4Core Clusters. Inorganic Chemistry, 2007, 46, 2159-2166.	4.0	22
36	New insights on the bridge carbonâ€"carbon bond in propellanes: A theoretical study based on the analysis of the electron localization function. Journal of Computational Chemistry, 2007, 28, 857-864.	3.3	47

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37	How the topological analysis of the electron localization function accounts for the inductive effect. Computational and Theoretical Chemistry, 2007, 811, 69-76.	1.5	13
38	New Findings on the Dielsâ˜'Alder Reactions. An Analysis Based on the Bonding Evolution Theory. Journal of Physical Chemistry A, 2006, 110, 13939-13947.	2.5	128
39	Electron localization function at the correlated level. Journal of Chemical Physics, 2006, 125, 024301.	3.0	135
40	The nature of the chemical bond in di- and polynuclear metal cluster complexes as depicted by the analysis of the electron localization function. Comptes Rendus Chimie, 2005, 8, 1400-1412.	0.5	36
41	Energetic and topological analyses of the oxidation reaction between Mon (n = 1, 2) and N2O. Journal of Computational Chemistry, 2005, 26, 1284-1293.	3.3	29
42	Charge-Shift Bondingâ€"A Class of Electron-Pair Bonds That Emerges from Valence Bond Theory and Is Supported by the Electron Localization Function Approach. Chemistry - A European Journal, 2005, 11, 6358-6371.	3.3	234
43	The Topological Analysis of the Electron Localization Function. A Key for a Position Space Representation of Chemical Bonds. Monatshefte FÃ¼r Chemie, 2005, 136, 855-879.	1.8	124
44	Theoretical Evaluation of Electron Delocalization in Aromatic Molecules by Means of Atoms in Molecules (AIM) and Electron Localization Function (ELF) Topological Approaches. Chemical Reviews, 2005, 105, 3911-3947.	47.7	661
45	Comparative Study of the Bonding in the First Series of Transition Metal 1:1 Complexes Mâ˜'L (M = Sc, ...,) Tj ETQq1 1 0.784314 rgBT	2.5	55
46	Energetic and topological analysis of the reaction of Mo and Mo2 with NH3, C2H2, and C2H4 molecules. Journal of Computational Chemistry, 2004, 25, 1647-1655.	3.3	15
47	Understanding the Molecular Mechanism of the 1,3-Dipolar Cycloaddition between Fulminic Acid and Acetylene in Terms of the Electron Localization Function and Catastrophe Theory. Chemistry - A European Journal, 2004, 10, 5165-5172.	3.3	95
48	A topological analysis of the proton transfer in the HFâ€" and HClâ€"(OH)â˜' interactions. Journal of Molecular Structure, 2004, 706, 3-6.	3.6	10
49	Topological analysis of the metal-support interaction: the case of Pd atoms on oxide surfaces. Chemical Physics Letters, 2004, 388, 132-138.	2.6	34
50	An Electron Localization Function Study of the Geometry of d0 Molecules of the Period 4 Metals Ca to Mn. Inorganic Chemistry, 2004, 43, 3248-3256.	4.0	61
51	How topological partitions of the electron distributions reveal delocalization. Physical Chemistry Chemical Physics, 2004, 6, 256-260.	2.8	143
52	Topological Analysis of the Reaction of Mn+(7S,5S) with H2O, NH3, and CH4Molecules. Journal of Physical Chemistry A, 2003, 107, 4862-4868.	2.5	65
53	Structure and Stability of Mâ˜'CO, M = First-Transition-Row Metal:â€‰ An Application of Density Functional Theory and Topological Approaches. Journal of Physical Chemistry A, 2003, 107, 4506-4514.	2.5	74
54	The Joint Use of Catastrophe Theory and Electron Localization Function to Characterize Molecular Mechanisms. A Density Functional Study of the Dielsâ˜'Alder Reaction between Ethylene and 1,3-Butadiene. Journal of Physical Chemistry A, 2003, 107, 6014-6024.	2.5	149

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55	The Spin-Pair Compositions as Local Indicators of the Nature of the Bonding. Journal of Physical Chemistry A, 2003, 107, 3081-3085.	2.5	143
56	The nature of the chemical bonding in the D3h and C2v isomers of Fe3(CO)12. New Journal of Chemistry, 2003, 27, 1049.	2.8	33
57	Topological Characterization of Three-Electron-Bonded Radical Anions. Journal of Physical Chemistry A, 2002, 106, 2561-2571.	2.5	24
58	Chemical Bonding in Hypervalent Molecules:â€‰ Is the Octet Rule Relevant?. Inorganic Chemistry, 2002, 41, 2164-2172.	4.0	131
59	Topological analysis of the bonds in incomplete cuboidal [Mo3S4] clusters. New Journal of Chemistry, 2002, 26, 844-850.	2.8	41
60	The synaptic order: a key concept to understand multicenter bonding. Journal of Molecular Structure, 2002, 614, 3-10.	3.6	283
61	Electron localization function studies of the nature of binding in neutral rare-gas containing hydrides: HKrCN, HKrNC, HXeCN, HXeNC, HXeOH, and HXeSH. Journal of Chemical Physics, 2001, 114, 4349.	3.0	33
62	Determination of substitutional sites in heterocycles from the topological analysis of the electron localization function (ELF). Journal of Computational Chemistry, 2000, 21, 509-514.	3.3	33
63	Determination of protonation sites in bases from topological rules. Chemical Physics, 2000, 252, 279-287.	1.9	67
64	Topological Analysis of the Electron Localization Function (ELF) Applied to the Electrophilic Aromatic Substitution. Journal of Physical Chemistry A, 2000, 104, 852-858.	2.5	171
65	Does the topological approach characterize the hydrogen bond?. Theoretical Chemistry Accounts, 2000, 104, 13-21.	1.4	235
66	Direct Space Representation of the Metallic Bond. Journal of Physical Chemistry A, 2000, 104, 947-953.	2.5	187
67	Synthesis and Characterization of [Cp2V(Î¼-Î·2:Î·4-butadiyne)ZrCpâ€˜2] Heterodimetallic Complexes (Cpâ€˜ =) Tj ETQq1 1 0.784314 gr Tetracoordinate Carbon (ptC). Organometallics, 2000, 19, 1901-1911.	2.3	60
68	Topological Analysis of the Electron Localization Function: A Help for Understanding the Complex Structure of Cryolitic Melts. Journal of the Electrochemical Society, 1999, 146, 2180-2183.	2.9	14
69	Bonding in hypohalous acids HOX (X=F, Cl, Br, and I) from the topological analysis of the electron localization function. Journal of Chemical Physics, 1999, 111, 2542-2555.	3.0	51
70	Computational tools for the electron localization function topological analysis. Computers & Chemistry, 1999, 23, 597-604.	1.2	805
71	Electron localization function comparative study of ground state, triplet state, radical anion, and cation in model carbonyl and imine compounds. Journal of Computational Chemistry, 1999, 20, 897-910.	3.3	45
72	Topological analysis of electron density in depleted homopolar chemical bonds. Journal of Computational Chemistry, 1999, 20, 1517-1526.	3.3	115

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73	Structure and Bonding of Chlorine Oxides and Peroxides:Â ClOx, ClOx-(x= 1â^'4), and Cl2Ox(x= 1â^'8). Journal of Physical Chemistry A, 1999, 103, 3078-3088.	2.5	74
74	Topological study, using a coupled ELF and catastrophe theory technique, of electron transfer in the Li+Cl2 system. New Journal of Chemistry, 1998, 22, 1341.	2.8	48
75	Characterization of Elementary Chemical Processes by Catastrophe Theory. Journal of Physical Chemistry A, 1997, 101, 7277-7282.	2.5	364
76	Importance of electrostatic interactions between nonbonded molecules in ice. Physical Review Letters, 1994, 73, 842-845.	7.8	24
77	The ELF Topological Analysis Contribution to Conceptual Chemistry and Phenomenological Models. , 0, , 141-162.		10
78	Isomerism in secondary bonded complexes: Do structural rules apply?. International Journal of Quantum Chemistry, 0, , e26670.	2.0	0
79	Electron group localization in atoms and molecules. Journal of Chemical Physics, 0, , .	3.0	2