Julien PilmÃ©

List of Publications by Year
in descending order

43 papers	1,030 citations	430874 18 h-index	434195 31 g-index
43 all docs	43 docs citations	43 times ranked	1353 citing authors

#	Article	IF	Citations
1	New insights in chemical reactivity from quantum chemical topology. Journal of Computational Chemistry, 2021, 42, 840-854.	3.3	10
2	Triggering Electron Transfer in Co(I) Dimers: Computational Evidences for a Reversible Disproportionation Mechanism. ChemPhysChem, 2021, 22, 788-795.	2.1	1
3	The Topological Analysis of the ELFx Localization Function: Quantitative Prediction of Hydrogen Bonds in the Guanineâ€“Cytosine Pair. Molecules, 2021, 26, 3336.	3.8	3
4	Astatine Facing Janus: Halogen Bonding vs. Charge-Shift Bonding. Molecules, 2021, 26, 4568.	3.8	3
5	Exploring The Sequence of Electron Density Along The Chemical Reactions Between Carbonyl Oxides And Ammonia/Water Using Bond Evolution Theory. ChemPhysChem, 2021, 22, 1792-1801.	2.1	10
6	â€¢OH oxidation of methionine in the presence of discrete water molecules: DFT, QTAIM and valence bond analyses. Structural Chemistry, 2020, 31, 719-730.	2.0	2
7	On the Interplay between Chargeâ€Shift Bonding and Halogen Bonding. ChemPhysChem, 2020, 21, 240-250.	2.1	18
8	Crystallographic structure and crystal field parameters in the [AnIV(DPA)3]2â^' series, An = Th, U, Np, Pu. Physical Chemistry Chemical Physics, 2020, 22, 14293-14308.	2.8	10
9	Quantum chemical topology at the spinâ€“orbit configuration interaction level: Application to astatine compounds. Journal of Computational Chemistry, 2020, 41, 2055-2065.	3.3	10
10	Quantum chemical topology from tight augmented core densities. Journal of Computational Chemistry, 2020, 41, 1616-1627.	3.3	0
11	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	3.3	113
12	Quantum Chemical Topology of the Electron Localization Function in the Field of Attosecond Electron Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 844-850.	4.6	17
13	Spinâ€“orbit coupling as a probe to decipher halogen bonding. Physical Chemistry Chemical Physics, 2018, 20, 29616-29624.	2.8	21
14	Understanding phase transition in the ZnSiP2 chalcopyrite, a quantum chemical topology study. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	6
15	The bonding picture in hypervalent XF₃ (Xâ€‰=â€‰Cl, Br, I, At) fluorides revisited with quantum chemical topology. Journal of Computational Chemistry, 2017, 38, 2753-2762.	3.3	11
16	Electron localization function from density components. Journal of Computational Chemistry, 2017, 38, 204-210.	3.3	19
17	211 At-labeled agents for alpha-immunotherapy: On the inÂvivo stability of astatine-agent bonds. European Journal of Medicinal Chemistry, 2016, 116, 156-164.	5.5	28
18	Quantum Chemical Topology in the Field of Quasirelativistic Quantum Calculations. Challenges and Advances in Computational Chemistry and Physics, 2016, , 553-582.	0.6	4

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19	What can tell the quantum chemical topology on carbonâ€“astatine bonds?. Molecular Physics, 2016, 114, 1326-1333.	1.7	11
20	Experimental and theoretical evidences of the influence of hydrogen bonding on the catalytic activity of a series of 2-hydroxy substituted quaternary ammonium salts in the styrene oxide/CO2 coupling reaction. Journal of Catalysis, 2016, 333, 29-39.	6.2	66
21	Toward an Understanding of the Oxidation Process of Methionine Enkephalin: A Combined Electrochemistry, Quantum Chemistry and Quantum Chemical Topology Analysis. Journal of Physical Chemistry B, 2015, 119, 6885-6893.	2.6	6
22	Electronic structures and geometries of the XF3 (X = Cl, Br, I, At) fluorides. Journal of Chemical Physics, 2015, 143, 114306.	3.0	17
23	Using the unusual weak Nâ€¦CO bond as a solvation probe. Molecular Simulation, 2014, 40, 185-195.	2.0	2
24	Phosphoryl Group as a Strong Ïƒ-Donor Anionic Phosphine-Type Ligand: A Combined Experimental and Theoretical Study on Long-Lived Room Temperature Luminescence of the [Ru(tpy)(bpy)(Ph₂PO)]⁺ Complex. Inorganic Chemistry, 2014, 53, 1946-1948.	4.0	25
25	Topological analyses of time-dependent electronic structures: application to electron-transfers in methionine enkephalin. Journal of Molecular Modeling, 2014, 20, 2368.	1.8	15
26	QTAIM Analysis in the Context of Quasirelativistic Quantum Calculations. Journal of Chemical Theory and Computation, 2014, 10, 4830-4841.	5.3	51
27	Probing Raman Enhancement in a Dopamineâ€“Ti₂O₄ Hybrid Using Stretched Molecular Geometries. Journal of Physical Chemistry A, 2014, 118, 1196-1202.	2.5	8
28	Quantum Chemical Topology Study of the Water-Platinum(II) Interaction. Inorganic Chemistry, 2013, 52, 1217-1227.	4.0	27
29	Introducing the ELF Topological Analysis in the Field of Quasirelativistic Quantum Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2985-2990.	5.3	43
30	Spinâ€driven activation of dioxygen in various metalloenzymes and their inspired models. Journal of Computational Chemistry, 2011, 32, 1178-1182.	3.3	14
31	New insights in quantum chemical topology studies using numerical gridâ€based analyses. Journal of Computational Chemistry, 2011, 32, 3207-3217.	3.3	47
32	Ligand Close Packing, Molecular Compactness, the Methyl Tilt, Molecular Conformations, and a New Model for the Anomeric Effect. Chemistry - A European Journal, 2010, 16, 3663-3675.	3.3	17
33	Reinterpretation of Three Crystal Structures of Alkali Oxoiodate(V) â€“ Description of the [I₃O₈]^{â€“}Anion and the Infinite 2D [I₃O₈^{â€“}]_{â^ž}Anion. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2010, 636, 1368-1379.	1.2	35
34	About the collapse of the 3.3â€‚Î¼m CH stretching band with ionization in polycyclic aromatic hydrocarbons: Configuration interaction and quantum Monte Carlo studies of the CH fragment. Journal of Chemical Physics, 2010, 133, 054301.	3.0	15
35	Regioselective N-alkylation of imidazo[4,5-b]pyridine-4-oxide derivatives: an experimental and DFT study. Tetrahedron Letters, 2009, 50, 1828-1833.	1.4	12
36	Advancing beyond charge analysis using the electronic localization function: Chemically intuitive distribution of electrostatic moments. Journal of Computational Chemistry, 2008, 29, 1440-1449.	3.3	60

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37	Unusual Bond Formation in Aspartic Protease Inhibitors: A Theoretical Study. Chemistry - A European Journal, 2007, 13, 5388-5393.	3.3	25
38	A possible 2,1â†'3,1 isomerization mechanism in zirconocene-catalyzed propene polymerization: An application of the density functional theory and combined ONIOM approach. Journal of Organometallic Chemistry, 2007, 692, 4227-4236.	1.8	12
39	A Topological Study of the Geometry of AF6E Molecules:Â Weak and Inactive Lone Pairs. Inorganic Chemistry, 2006, 45, 6198-6204.	4.0	27
40	Comments on the nature of the bonding in oxygenated dinuclear copper enzyme models. Computational and Theoretical Chemistry, 2006, 764, 77-86.	1.5	19
41	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 /O	2.5	55
42	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
43	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