Maurizio Sironi

List of Publications by Year
in descending order

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63	1,373	279798	361022
papers	citations	23	35
		h-index	g-index

63	63	63	1498
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Halogen bonding in ligandâ€“receptor systems in the framework of classical force fields. Physical Chemistry Chemical Physics, 2011, 13, 19508.	2.8	85
2	Halogen bonds with benzene: An assessment of DFT functionals. Journal of Computational Chemistry, 2014, 35, 386-394.	3.3	73
3	Molecular dynamics simulation of aqueous solutions of trimethylamine-N-oxide and tert-butyl alcohol. Physical Chemistry Chemical Physics, 2003, 5, 4905.	2.8	69
4	Determination of extremely localized molecular orbitals and their application to quantum mechanics/molecular mechanics methods and to the study of intramolecular hydrogen bonding. Computational and Theoretical Chemistry, 2003, 632, 157-172.	1.5	67
5	Expansion of the spin-coupled wavefunction in Slater determinants. Theoretica Chimica Acta, 1993, 85, 261-270.	0.8	61
6	Extremely localized molecular orbitals: theory and applications. Theoretical Chemistry Accounts, 2007, 117, 685-698.	1.4	60
7	Halogenâ€Bonding Interactions with Ï€ Systems: CCSD(T), MP2, and DFT Calculations. ChemPhysChem, 2012, 13, 4224-4234.	2.1	51
8	In silico design of tubulin-targeted antimitotic peptides. Nature Chemistry, 2009, 1, 642-648.	13.6	38
9	The Extraordinary Electronic Structure of N2S2. Journal of the American Chemical Society, 1996, 118, 6472-6476.	13.7	36
10	Synthesis, Crystal Structure and Biological Activity of 2-Hydroxyethylammonium Salt of p-Aminobenzoic Acid. PLoS ONE, 2014, 9, e101892.	2.5	36
11	A novel extremely localized molecular orbitals based technique for the one-electron density matrix computation. Chemical Physics Letters, 2005, 415, 256-260.	2.6	35
12	Hartreeâ€“Fock limit properties of the water dimer in absence of BSSE. Chemical Physics, 1998, 232, 275-287.	1.9	33
13	Boehmeriasin A as new lead compound for the inhibition of topoisomerases and SIRT2. European Journal of Medicinal Chemistry, 2015, 92, 766-775.	5.5	32
14	A novel approach to relax extremely localized molecular orbitals: the extremely localized molecular orbital?valence bond method. Theoretical Chemistry Accounts, 2004, 112, 254.	1.4	31
15	Studies on Umami Taste. Synthesis of New Guanosine 5â€²-Phosphate Derivatives and Their Synergistic Effect with Monosodium Glutamate. Journal of Agricultural and Food Chemistry, 2008, 56, 1043-1050.	5.2	31
16	Optimal virtual orbitals to relax wave functions built up with transferred extremely localized molecular orbitals. Journal of Computational Chemistry, 2005, 26, 827-835.	3.3	30
17	Solvent effect on halogen bonding: The case of the Iâ‹¯O interaction. Journal of Molecular Graphics and Modelling, 2012, 38, 31-39.	2.4	30
18	Molecular dynamics simulation of aqueous solutions of glycine betaine. Chemical Physics Letters, 2003, 367, 238-244.	2.6	29

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19	The electronic structure of CH2 and the cycloaddition reaction of methylene with ethene. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 1651.	1.1	28
20	DENPOL: A new program to determine electron densities of polypeptides using extremely localized molecular orbitals. Computational and Theoretical Chemistry, 2009, 898, 8-16.	1.5	27
21	Quinazolinecarboline alkaloid evodiamine as scaffold for targeting topoisomerase I and sirtuins. Bioorganic and Medicinal Chemistry, 2013, 21, 6920-6928.	3.0	26
22	On the suitability of strictly localized orbitals for hybrid QM/MM calculations. Journal of Computational Chemistry, 2006, 27, 515-523.	3.3	25
23	4-(1,2-diarylbut-1-en-1-yl)isobutyranilide derivatives as inhibitors of topoisomerase II. European Journal of Medicinal Chemistry, 2016, 118, 79-89.	5.5	24
24	A Simple Mechanism Underlying the Effect of Protecting Osmolytes on Protein Folding. Journal of Chemical Theory and Computation, 2011, 7, 3846-3852.	5.3	23
25	The modern valence bond description of naphthalene. Journal of the Chemical Society Chemical Communications, 1989, , 675.	2.0	22
26	Frozen core orbitals as an alternative to specific frontier bond potential in hybrid Quantum Mechanics/Molecular Mechanics methods. Chemical Physics Letters, 2006, 427, 236-240.	2.6	22
27	Metadynamics Study of a Î²-Hairpin Stability in Mixed Solvents. Journal of the American Chemical Society, 2011, 133, 2897-2903.	13.7	22
28	Electrophysiological and metabolic effects of CHF5074 in the hippocampus: Protection against in vitro ischemia. Pharmacological Research, 2014, 81, 83-90.	7.1	22
29	Unusual properties of aqueous solutions of l-proline: A molecular dynamics study. Chemical Physics Letters, 2005, 415, 274-278.	2.6	20
30	The nature of the platinumâ€“phosphine bond. An ab initio Hartreeâ€“Fock and density functional study. Journal of the Chemical Society Dalton Transactions, 1995, , 4121-4126.	1.1	18
31	Camptothecinâ€7â€ylâ€methanthiole: Semisynthesis and Biological Evaluation. ChemMedChem, 2012, 7, 2134-2143.	3.2	18
32	Water interaction with glycine betaine: A hybrid QM/MM molecular dynamics simulation. Physical Chemistry Chemical Physics, 2001, 3, 1081-1085.	2.8	17
33	X-ray constrained spin-coupled technique: theoretical details and further assessment of the method. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 778-797.	0.1	17
34	The spin-coupled description of lithium clusters. Computational and Theoretical Chemistry, 1992, 259, 383-410.	1.5	15
35	Regio- and diastereoselectivity in TiCl4-promoted reduction of 2-aryl-substituted cis-4-methyl-5-trifluoromethyl-1,3-dioxolanes. Tetrahedron: Asymmetry, 2002, 13, 2609-2618.	1.8	14
36	Synthesis of Pironetinâ€“Dumetorine Hybrids as Tubulin Binders. European Journal of Organic Chemistry, 2016, 2016, 2029-2036.	2.4	14

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37	The transferability of extremely localized molecular orbitals. Computational and Theoretical Chemistry, 2000, 529, 47-54.	1.5	13
38	A Hylleraas functional based perturbative technique to relax the extremely localized molecular orbital wavefunction. Journal of Chemical Physics, 2008, 129, 054101.	3.0	13
39	Ab initio non-orthogonal approaches to the computation of weak interactions and of localised molecular orbitals for QM/MM procedures. Computational and Theoretical Chemistry, 2001, 573, 25-42.	1.5	11
40	The unusual coordination of carbon atoms in bicyclic l,6-methano[10]annulene: a modern valence bond study. Computational and Theoretical Chemistry, 1995, 338, 257-265.	1.5	9
41	Evidence for a nucleophilic anti-attack on the cleaved C(2)â€“oxygen bond in Cl2AlH-catalyzed ring-opening of 2-substituted 1,3-dioxolanes. Tetrahedron Letters, 2005, 46, 1837-1840.	1.4	9
42	Modeling enzymatic processes: A molecular simulation analysis of the origins of regioselectivity. Chemical Physics Letters, 2006, 418, 373-376.	2.6	9
43	Atomic level description of the protecting effect of osmolytes against thermal denaturation of proteins. Chemical Physics Letters, 2007, 438, 298-303.	2.6	9
44	Vinblastine perturbation of tubulin protofilament structure: a computational insight. Physical Chemistry Chemical Physics, 2010, 12, 15530.	2.8	9
45	In silico study of VP35 inhibitors: from computational alanine scanning to essential dynamics. Molecular BioSystems, 2015, 11, 2152-2157.	2.9	9
46	Effects of hydrated Mg++ interacting with the guanine site in cytosineâ€“guanine nucleic acidâ€“base pair: an ab initio Hartreeâ€“Fock study in the absence of basis set superposition error. Computational and Theoretical Chemistry, 2000, 529, 209-217.	1.5	8
47	Determination of extremely localized molecular orbitals in the framework of density functional theory. Theoretical Chemistry Accounts, 2004, 112, 247.	1.4	8
48	Computer aided design of FtsZ targeting oligopeptides. RSC Advances, 2013, 3, 1739-1743.	3.6	8
49	Molecular modeling of the inhibition of proteinâ€“protein interactions with small molecules: The IL2â€“IL2Rî± case. Chemical Physics Letters, 2011, 517, 217-222.	2.6	7
50	9â€Fluorenoneâ€2â€Carboxylic Acid as a Scaffold for Tubulin Interacting Compounds. ChemPlusChem, 2013, 78, 663-669.	2.8	7
51	Spin-coupled VB study of the di-cations of methane, ammonia and water. Molecular Physics, 1988, 65, 251-259.	1.7	6
52	New ab initio VB interaction potential for molecular dynamics simulation of liquid water. Advances in Quantum Chemistry, 1998, 32, 263-284.	0.8	6
53	Accurate Description of Nitrogenous Base Flexibility in Classical Molecular Dynamics Simulations of Nucleotides Bound to Proteins. Journal of Physical Chemistry B, 2007, 111, 6297-6302.	2.6	6
54	Molecular insights into the stabilization of proteinâ€“protein interactions with small molecule: The FKBP12â€“rapamycinâ€“FRB case study. Chemical Physics Letters, 2013, 587, 68-74.	2.6	6

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55	Modelling the effect of osmolytes on peptide mechanical unfolding. Chemical Physics Letters, 2013, 578, 138-143.	2.6	5
56	A valence bond description of the bromine halogen bond. International Journal of Quantum Chemistry, 2019, 119, e25946.	2.0	4
57	A molecular dynamics study of human endostatin and its synthetic fragments with antiangiogenic properties. Physical Chemistry Chemical Physics, 2006, 8, 3066.	2.8	3
58	Computational investigation of the nucleophilic reaction between methylthiolate and 4-bromo-3-methylamino-isothiazole 1,1-dioxide. Computational and Theoretical Chemistry, 2005, 726, 107-113.	1.5	2
59	A molecular dynamics study of an endostatin-derived peptide with antiangiogenic activity and of its mutants. Chemical Physics Letters, 2008, 455, 311-315.	2.6	2
60	Simulating Multiple Substrate-Binding Events by Î³-Glutamyltransferase Using Accelerated Molecular Dynamics. Journal of Physical Chemistry B, 2020, 124, 10104-10116.	2.6	2
61	Exploring Orthogonality between Halogen and Hydrogen Bonding Involving Benzene. Molecules, 2021, 26, 7126.	3.8	1
62	Spin correlation function of benzene and naphthalene from spin-coupled wave functions. Journal of Chemical Physics, 2001, 114, 1505-1509.	3.0	0
63	Molecular Similarity Perception Based on Machine-Learning Models. International Journal of Molecular Sciences, 2022, 23, 6114.	4.1	0