# Maurizio Sironi

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/393650/publications.pdf

Version: 2024-02-01

| 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 | Molecular Similarity Perception Based on Machine-Learning Models. International Journal of Molecular Sciences, 2022, 23, 6114. | 4.1 | 0 |
| 2 | Exploring Orthogonality between Halogen and Hydrogen Bonding Involving Benzene. Molecules, 2021, 26, 7126. | 3.8 | 1 |
| 3 | Simulating Multiple Substrate-Binding Events by Î³-Glutamyltransferase Using Accelerated Molecular Dynamics. Journal of Physical Chemistry B, 2020, 124, 10104-10116. | 2.6 | 2 |
| 4 | 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 |
| 5 | A valence bond description of the bromine halogen bond. International Journal of Quantum Chemistry, 2019, 119, e25946. | 2.0 | 4 |
| 6 | Synthesis of Pironetinâ€“Dumetorine Hybrids as Tubulin Binders. European Journal of Organic Chemistry, 2016, 2016, 2029-2036. | 2.4 | 14 |
| 7 | 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 |
| 8 | 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 |
| 9 | In silico study of VP35 inhibitors: from computational alanine scanning to essential dynamics. Molecular BioSystems, 2015, 11, 2152-2157. | 2.9 | 9 |
| 10 | Halogen bonds with benzene: An assessment of DFT functionals. Journal of Computational Chemistry, 2014, 35, 386-394. | 3.3 | 73 |
| 11 | Electrophysiological and metabolic effects of CHF5074 in the hippocampus: Protection against in vitro ischemia. Pharmacological Research, 2014, 81, 83-90. | 7.1 | 22 |
| 12 | Synthesis, Crystal Structure and Biological Activity of 2-Hydroxyethylammonium Salt of p-Aminobenzoic Acid. PLoS ONE, 2014, 9, e101892. | 2.5 | 36 |
| 13 | Computer aided design of FtsZ targeting oligopeptides. RSC Advances, 2013, 3, 1739-1743. | 3.6 | 8 |
| 14 | 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 |
| 15 | Quinazolinecarboline alkaloid evodiamine as scaffold for targeting topoisomerase I and sirtuins. Bioorganic and Medicinal Chemistry, 2013, 21, 6920-6928. | 3.0 | 26 |
| 16 | Modelling the effect of osmolytes on peptide mechanical unfolding. Chemical Physics Letters, 2013, 578, 138-143. | 2.6 | 5 |
| 17 | 9â€Fluorenoneâ€2â€Carboxylic Acid as a Scaffold for Tubulin Interacting Compounds. ChemPlusChem, 2013, 78, 663-669. | 2.8 | 7 |
| 18 | Camptothecinâ€7â€ylâ€methanthiole: Semisynthesis and Biological Evaluation. ChemMedChem, 2012, 7, 2134-2143. | 3.2 | 18 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Halogenâ€Bonding Interactions with Ï€ Systems: CCSD(T), MP2, and DFT Calculations. ChemPhysChem, 2012, 13, 4224-4234. | 2.1 | 51 |
| 20 | 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 |
| 21 | Metadynamics Study of a Î²-Hairpin Stability in Mixed Solvents. Journal of the American Chemical Society, 2011, 133, 2897-2903. | 13.7 | 22 |
| 22 | Halogen bonding in ligandâ€“receptor systems in the framework of classical force fields. Physical Chemistry Chemical Physics, 2011, 13, 19508. | 2.8 | 85 |
| 23 | 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 |
| 24 | Molecular modeling of the inhibition of proteinâ€“protein interactions with small molecules: The IL2â€“IL2Rβ± case. Chemical Physics Letters, 2011, 517, 217-222. | 2.6 | 7 |
| 25 | Vinblastine perturbation of tubulin protofilament structure: a computational insight. Physical Chemistry Chemical Physics, 2010, 12, 15530. | 2.8 | 9 |
| 26 | In silico design of tubulin-targeted antimitotic peptides. Nature Chemistry, 2009, 1, 642-648. | 13.6 | 38 |
| 27 | 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 |
| 28 | 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 |
| 29 | 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 |
| 30 | A Hylleraas functional based perturbative technique to relax the extremely localized molecular orbital wavefunction. Journal of Chemical Physics, 2008, 129, 054101. | 3.0 | 13 |
| 31 | 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 |
| 32 | Atomic level description of the protecting effect of osmolytes against thermal denaturation of proteins. Chemical Physics Letters, 2007, 438, 298-303. | 2.6 | 9 |
| 33 | Extremely localized molecular orbitals: theory and applications. Theoretical Chemistry Accounts, 2007, 117, 685-698. | 1.4 | 60 |
| 34 | A molecular dynamics study of human endostatin and its synthetic fragments with antiangiogenic properties. Physical Chemistry Chemical Physics, 2006, 8, 3066. | 2.8 | 3 |
| 35 | Modeling enzymatic processes: A molecular simulation analysis of the origins of regioselectivity. Chemical Physics Letters, 2006, 418, 373-376. | 2.6 | 9 |
| 36 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | On the suitability of strictly localized orbitals for hybrid QM/MM calculations. Journal of Computational Chemistry, 2006, 27, 515-523. | 3.3 | 25 |
| 38 | 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 |
| 39 | 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 |
| 40 | Unusual properties of aqueous solutions of l-proline: A molecular dynamics study. Chemical Physics Letters, 2005, 415, 274-278. | 2.6 | 20 |
| 41 | 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 |
| 42 | 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 |
| 43 | 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 |
| 44 | Determination of extremely localized molecular orbitals in the framework of density functional theory. Theoretical Chemistry Accounts, 2004, 112, 247. | 1.4 | 8 |
| 45 | Molecular dynamics simulation of aqueous solutions of glycine betaine. Chemical Physics Letters, 2003, 367, 238-244. | 2.6 | 29 |
| 46 | 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 |
| 47 | Molecular dynamics simulation of aqueous solutions of trimethylamine-N-oxide and tert-butyl alcohol. Physical Chemistry Chemical Physics, 2003, 5, 4905. | 2.8 | 69 |
| 48 | 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 |
| 49 | Spin correlation function of benzene and naphthalene from spin-coupled wave functions. Journal of Chemical Physics, 2001, 114, 1505-1509. | 3.0 | 0 |
| 50 | Water interaction with glycine betaine: A hybrid QM/MM molecular dynamics simulation. Physical Chemistry Chemical Physics, 2001, 3, 1081-1085. | 2.8 | 17 |
| 51 | 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 |
| 52 | The transferability of extremely localized molecular orbitals. Computational and Theoretical Chemistry, 2000, 529, 47-54. | 1.5 | 13 |
| 53 | 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 |
| 54 | Hartreeâ€“Fock limit properties of the water dimer in absence of BSSE. Chemical Physics, 1998, 232, 275-287. | 1.9 | 33 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | New ab initio VB interaction potential for molecular dynamics simulation of liquid water. Advances in Quantum Chemistry, 1998, 32, 263-284. | 0.8 | 6 |
| 56 | The Extraordinary Electronic Structure of N2S2. Journal of the American Chemical Society, 1996, 118, 6472-6476. | 13.7 | 36 |
| 57 | 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 |
| 58 | 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 |
| 59 | Expansion of the spin-coupled wavefunction in Slater determinants. Theoretica Chimica Acta, 1993, 85, 261-270. | 0.8 | 61 |
| 60 | The spin-coupled description of lithium clusters. Computational and Theoretical Chemistry, 1992, 259, 383-410. | 1.5 | 15 |
| 61 | The modern valence bond description of naphthalene. Journal of the Chemical Society Chemical Communications, 1989, , 675. | 2.0 | 22 |
| 62 | Spin-coupled VB study of the di-cations of methane, ammonia and water. Molecular Physics, 1988, 65, 251-259. | 1.7 | 6 |
| 63 | 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 |