Caterina Ghio

List of Publications by Year
in descending order

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107 papers	7,374 citations	147801 31 h-index	53230 85 g-index
111 all docs	111 docs citations	111 times ranked	5237 citing authors

#	Article	IF	Citations
1	A new force field for molecular mechanical simulation of nucleic acids and proteins. Journal of the American Chemical Society, 1984, 106, 765-784.	13.7	4,802
2	Theoretical calculations on 1,2-ethanediol. Gauche-trans equilibrium in gas-phase and aqueous solution. Journal of the American Chemical Society, 1991, 113, 6719-6729.	13.7	97
3	Quantum mechanical and molecular mechanical studies on a model for the dihydroxyacetone phosphate-glyceraldehyde phosphate isomerization catalyzed by triose phosphate isomerase (TIM). Journal of the American Chemical Society, 1984, 106, 3623-3632.	13.7	86
4	Ab initio studies of free and monohydrated carboxylic acids in the gas phase. The Journal of Physical Chemistry, 1994, 98, 486-493.	2.9	73
5	Do Enzymes Stabilize Transition States by Electrostatic Interactions or pKa Balance: The Case of Triose Phosphate Isomerase (TIM)?. Journal of the American Chemical Society, 1995, 117, 9855-9862.	13.7	72
6	Olefin Insertion into the Rhodiumâ˜Hydrogen Bond as the Step Determining the Regioselectivity of Rhodium-Catalyzed Hydroformylation of Vinyl Substrates:Â Comparison between Theoretical and Experimental Results. Organometallics, 2001, 20, 5394-5404.	2.3	67
7	Theoretical calculations on 1,2-ethanediol. 2. Equilibrium of the gauche conformers with and without an intramolecular hydrogen bond in aqueous solution. Journal of the American Chemical Society, 1992, 114, 4752-4758.	13.7	66
8	Theoretical Studies on the Conformation of Protonated Dopamine in the Gas Phase and in Aqueous Solution. Journal of the American Chemical Society, 1999, 121, 4804-4815.	13.7	64
9	Monte Carlo simulation studies of the solvation of ions. 1. Acetate anion and methylammonium cation. Journal of the American Chemical Society, 1986, 108, 185-191.	13.7	60
10	An appraisal of solvation effects on chemical functional groups: The amidic and the esteric linkages. Computational and Theoretical Chemistry, 1990, 204, 253-283.	1.5	60
11	Theoretical Conformational Analysis for Neurotransmitters in the Gas Phase and in Aqueous Solution. Norepinephrine. Journal of the American Chemical Society, 2003, 125, 2770-2785.	13.7	58
12	Theoretical studies of the 2- and 4-hydroxybenzoic acid with competing hydrogen bonds in the gas phase and aqueous solution. The Journal of Physical Chemistry, 1993, 97, 4628-4642.	2.9	57
13	Monte Carlo simulation studies of the solvation of ions. 2. Glycine zwitterion. Computational and Theoretical Chemistry, 1988, 166, 385-392.	1.5	56
14	Ketoâ€enol tautomerism in linear and cyclic Î²â€diketones: A DFT study in vacuo and in solution. International Journal of Quantum Chemistry, 2008, 108, 1840-1855.	2.0	53
15	Plicatin B conformational landscape and affinity to copper (I and II) metal cations. A DFT study. Physical Chemistry Chemical Physics, 2009, 11, 776-790.	2.8	51
16	The catalytic effect of water on the ketoâ€“enol tautomerism. Pyruvate and acetylacetone: a computational challenge. Physical Chemistry Chemical Physics, 2010, 12, 10173.	2.8	51
17	Theoretical Investigation of Tautomeric Equilibria for Isonicotinic Acid, 4-Pyridone, and Acetylacetone in Vacuo and in Solution. Journal of Chemical Theory and Computation, 2007, 3, 1249-1266.	5.3	48
18	Antioxidant Properties of Pterocarpans through Their Copper(II) Coordination Ability. A DFT Study in Vacuo and in Aqueous Solution. Journal of Physical Chemistry A, 2009, 113, 15206-15216.	2.5	48

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19	Bifurcated vs. linear hydrogen bonds: dimethyl phosphate and formate anion interactions with water. Journal of the American Chemical Society, 1983, 105, 5226-5230.	13.7	47
20	Monte Carlo simulations of the solvation of the dimethyl phosphate anion. Journal of the American Chemical Society, 1985, 107, 2229-2239.	13.7	47
21	Theoretical Investigations on the Structure of Poly(iminomethylenes) with Aliphatic Side Chains. Conformational Studies and Comparison with Experimental Spectroscopic Data. Journal of the American Chemical Society, 1997, 119, 1059-1071.	13.7	45
22	Simple model for the effect of Glu165 â†' Asp165 mutation on the rate of catalysis in triose phosphate isomerase. Journal of Molecular Biology, 1986, 191, 23-27.	4.2	44
23	The effect of ?full? and ?limited? counterpoise corrections with different basis sets on the energy and the equilibrium distance of hydrogen bonded dimers. International Journal of Quantum Chemistry, 1987, 32, 207-226.	2.0	44
24	The protonation of three-membered ring molecules Theab initio SCF versus the electrostatic picture of the proton approach. Theoretica Chimica Acta, 1973, 30, 151-158.	0.8	42
25	On a semiclassical interpretation of inter- and intramolecular interactions. International Journal of Quantum Chemistry, 1984, 26, 637-686.	2.0	41
26	Interplay of intra- and intermolecular H-bonds for the addition of a water molecule to the neutral and N-protonated forms of noradrenaline. International Journal of Quantum Chemistry, 2002, 90, 641-656.	2.0	38
27	Quantum Mechanical Study of Stereoselectivity in the Oxazaborolidine-Catalyzed Reduction of Acetophenone. Journal of the American Chemical Society, 2003, 125, 10027-10039.	13.7	37
28	The influence of the basis set on the evaluation of conformational energies for small organic solutes in aqueous solutions. Computational and Theoretical Chemistry, 1986, 137, 263-277.	1.5	34
29	Conformational properties of ethanediol in aqueous solution as described by the continuous model of the solvent. Computational and Theoretical Chemistry, 1992, 254, 287-300.	1.5	34
30	Investigation of alkyl metal intermediate formation in the rhodium-catalyzed hydroformylation: Experimental and theoretical approaches. Coordination Chemistry Reviews, 2010, 254, 696-706.	18.8	33
31	The decomposition of the SCF interaction energy in hydrogen bonded dimers corrected for basis set superposition errors: An examination of the basis set dependence. International Journal of Quantum Chemistry, 1987, 32, 227-248.	2.0	31
32	Effect of counterpoise corrections on the components of the interaction energy in the formate-, acetate-, and phosphate-water dimers: a study of basis set effects. The Journal of Physical Chemistry, 1989, 93, 5401-5410.	2.9	31
33	The effect of intramolecular H-bonds on the aqueous solution continuum description of the N-protonated form of dopamine. Chemical Physics, 1996, 204, 239-249.	1.9	31
34	Appraisal of solvation effects on chemical functional groups: amides and esters in terms of transferable subgroup contributions. Journal of the American Chemical Society, 1989, 111, 3417-3421.	13.7	30
35	Competitive H-bonds in vacuo and in aqueous solution for N-protonated adrenaline and its monohydrated complexes. Computational and Theoretical Chemistry, 2007, 811, 223-240.	1.5	30
36	Semiclassical models in theoretical chemistry. Some results and future prospects. Computational and Theoretical Chemistry, 1986, 135, 39-66.	1.5	29

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37	Theoretical Studies on the Relative Stability of Neutral and Protonated N,N'-Diarylguanidines in Aqueous Solution Using Continuum Solvent Models. The Journal of Physical Chemistry, 1994, 98, 5422-5430.	2.9	29
38	The effect of diffuse functions on minimal basis set superposition errors for H-bonded dimers. Journal of Computational Chemistry, 1990, 11, 930-942.	3.3	28
39	The Effect of Intramolecular Interactions on the Transferability Properties of Localized Descriptions of Chemical Groups. Israel Journal of Chemistry, 1980, 19, 109-126.	2.3	26
40	Ab Initio Investigation of the Methylimidazoleâ^'Indole Complexes as Models of the Histidineâ^'Tryptophan Pair. Journal of Physical Chemistry A, 1998, 102, 6152-6160.	2.5	26
41	Towards a unified view of the description of internal and external fields acting on chemical functional groups. Pure and Applied Chemistry, 1988, 60, 231-244.	1.9	25
42	Force field parameters for molecular mechanical simulation of dehydroamino acid residues. Journal of Computational Chemistry, 1991, 12, 934-942.	3.3	25
43	Theoretical Conformational Analysis for Neurotransmitters in the Gas Phase and in Aqueous Solution. Serotonin. Journal of Chemical Theory and Computation, 2005, 1, 801-816.	5.3	24
44	Basis set superposition errors and counterpoise corrections for some basis sets evaluated for a few X-.cntdot..cntdot..cntdot.M dimers. The Journal of Physical Chemistry, 1990, 94, 2267-2273.	2.9	23
45	Conformational Landscape of (R,R)-Pterocarpans with Biological Activity in Vacuo and in Aqueous Solution (PCM and/or Water Clusters)â€. Journal of Physical Chemistry A, 2006, 110, 647-659.	2.5	23
46	Theoretical calculations on the 1:1 complexes of N-aromatics with water. Computational and Theoretical Chemistry, 1989, 187, 219-232.	1.5	21
47	Caco-2 cell permeability modelling: a neural network coupled genetic algorithm approach. Journal of Computer-Aided Molecular Design, 2007, 21, 207-221.	2.9	20
48	Comparative study of imidazole hydration:Ab initioand electrostatic calculations vs. Cambridge structural database analysis. Journal of Computational Chemistry, 1990, 11, 1038-1046.	3.3	19
49	Monte carlo simulation studies of the solvation of ions. 3. The non intramolecularly H-bonded form of glycine zwitterion.. Journal of Molecular Liquids, 1990, 47, 139-160.	4.9	19
50	Computational prediction of the regio- and diastereoselectivity in a rhodium-catalyzed hydroformylation/cyclization domino process. Journal of Molecular Modeling, 2007, 13, 823-837.	1.8	19
51	The role of electrostatics in solute-solvent interactions with the continuum. Computational and Theoretical Chemistry, 1992, 256, 187-216.	1.5	18
52	Noncovalent interactions of medium strength. A revised interpretation and examples of its applications. International Journal of Quantum Chemistry, 1989, 35, 223-239.	2.0	17
53	5-fluorouracil dimers in aqueous solution: molecular dynamics in water and continuum solvation. International Journal of Quantum Chemistry, 2002, 88, 133-146.	2.0	17
54	Theoretical studies on the effects of methods and parameterization on the calculated free energy of hydration for small molecules. International Journal of Quantum Chemistry, 2004, 99, 161-178.	2.0	17

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55	Markedly different selectivity in the rhodium catalyzed hydroformylation of vinyl olefins containing a chiral alkoxy or alkyl group: good agreement between theory and experiment. Inorganica Chimica Acta, 2004, 357, 2980-2988.	2.4	17
56	Ab Initio and Density Functional Evaluations of the Molecular Conformations of Î²-Caryophyllene and 6-Hydroxycaryophyllene. Journal of Organic Chemistry, 2000, 65, 6910-6916.	3.2	16
57	Basis set superposition errors for Slater vs. gaussian basis functions in H-bond interactions. Computational and Theoretical Chemistry, 1995, 330, 77-83.	1.5	15
58	Theoretical investigation of histidine-tryptophan preferential interactions. Theoretical Chemistry Accounts, 1999, 101, 143-150.	1.4	15
59	Alkyl-rhodium transition state stabilities as a tool to predict regio- and stereoselectivity in the hydroformylation of chiral substrates. Journal of Organometallic Chemistry, 2005, 690, 2339-2350.	1.8	15
60	A Reappraisal of the Hydrogen Bonding Interaction Obtained by Combining Energy Decomposition Analyses and Counterpoise Corrections. Topics in Molecular Organization and Engineering, 1988, , 507-559.	0.1	15
61	The effect of substitution on the properties of a chemical group. Theoretica Chimica Acta, 1978, 50, 117-134.	0.8	14
62	Neutral organic lewis acids of ? type. International Journal of Quantum Chemistry, 1986, 29, 527-539.	2.0	14
63	Protonated serotonin conformational landscape in vacuo and in aqueous solution (IEF-PCM): Role of correlation effects and monohydration. Computational and Theoretical Chemistry, 2006, 769, 123-134.	1.5	14
64	The effect of substitution on the properties of a chemical group. Theoretica Chimica Acta, 1980, 56, 61-73.	0.8	13
65	Ab initio relative stability of a few conformers of bilirubinin vacuo and in aqueous solution (PCM). International Journal of Quantum Chemistry, 1998, 70, 395-405.	2.0	13
66	Theoretical Studies on the Continuum Solvation of SomeN,Nâ€˜-Dimethyl- andN-Methyl,Nâ€˜-acetyl-Guanidine and Guanidinium Conformers. Journal of Physical Chemistry A, 1999, 103, 1857-1867.	2.5	13
67	B3LYP/6-31G* conformational landscape in vacuo of some pterocarpan stereoisomers with biological activity. Physical Chemistry Chemical Physics, 2004, 6, 2849.	2.8	13
68	The effect of substitution on the properties of a chemical group. Theoretica Chimica Acta, 1980, 56, 75-87.	0.8	12
69	On the acidic properties of compounds with Cî—»C or Nî—»N electrophilic double bonds. Computational and Theoretical Chemistry, 1986, 135, 299-328.	1.5	12
70	Stability and acidity of salicylic acid rotamers in aqueous solution. A continuous model study. Journal of Molecular Liquids, 1994, 61, 1-16.	4.9	12
71	The effect of small substituents on the properties of indole. An ab initio 6-31G* study. Computational and Theoretical Chemistry, 1998, 433, 203-216.	1.5	12
72	Continuum solvent effects on various isomers of bilirubin. Physical Chemistry Chemical Physics, 2000, 2, 4884-4890.	2.8	12

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73	Ab initio modeling of competitive drug-drug interactions: 5-fluorouracil dimers in the gas phase and in solution. International Journal of Quantum Chemistry, 2001, 83, 128-142.	2.0	11
74	The intramolecular mechanism for the second proton transfer in triosephosphate isomerase (TIM): A QM/FE approach. Journal of Computational Chemistry, 2003, 24, 46-56.	3.3	11
75	Computational Results Provide a Synthetically Unprecedented Explanation for the Î²-Regioselectivity in the Rh-Catalyzed Hydroformylation of Vinylidenic Substrates. European Journal of Inorganic Chemistry, 2009, 2009, 98-103.	2.0	11
76	Structure and Dynamics of the Hydrogen-Bond Network around (R,R)-Pterocarpans with Biological Activity in Aqueous Solution. Journal of Physical Chemistry B, 2005, 109, 16918-16925.	2.6	10
77	Rhodium-catalyzed deuterioformylation of the ketal-masked Î²-isophorone: Evidence for a tertiary alkyl rhodium intermediate as a precursor of the main reaction product acetaldehyde derivative. Inorganica Chimica Acta, 2009, 362, 1641-1644.	2.4	10
78	An analysis of the interaction energy in some SN2 reactions. Theoretica Chimica Acta, 1981, 60, 79-87.	0.8	9
79	Theoretical investigation on the oxazaborolidine-ketone interaction in small model systems. Theoretical Chemistry Accounts, 2004, 111, 287-302.	1.4	9
80	Dependence of the wittig reaction mechanism on the environment and on the substituents at the aldehyde group and at the phosphonium ylide. International Journal of Quantum Chemistry, 2010, 110, 765-776.	2.0	9
81	Cation migration between two unequivalent sites in 4-cyano pyridine alkali metal ion pairs. Chemical Physics, 1978, 31, 31-37.	1.9	8
82	Molecular interactions in a homogeneous electric field: the (HF)2 complex. Theoretica Chimica Acta, 1993, 85, 167-187.	0.8	8
83	Chemical reaction mechanisms in vacuo, in solution and in enzyme fields: isomerization catalyzed by triose phosphate isomerase (TIM). Computational and Theoretical Chemistry, 1996, 371, 287-298.	1.5	8
84	Ab initio study of preferential interactions between aromatic side chains. International Journal of Quantum Chemistry, 1999, 73, 175-186.	2.0	8
85	Basis Set, Level, and Continuum Solvation Effects on the Stability of a Synthetic Dipeptide:Â PIDOTIMOD. Journal of Physical Chemistry A, 1999, 103, 5823-5832.	2.5	8
86	Ab initio explorative survey of the mechanism catalyzed by mandelate racemase. Computational and Theoretical Chemistry, 1997, 390, 217-223.	1.5	7
87	A theoretical study on reaction pathways to carbanions. Computers & Chemistry, 2000, 24, 311-324.	1.2	6
88	Cholic Acid Derivatives Containing Both 2-Naphthylcarbamate and 3,5-Dinitrophenylcarbamate Groups:Â A Combined Circular Dichroismâ^'Molecular Mechanics Approach to the Definition of Their Molecular Conformation. Journal of Organic Chemistry, 2003, 68, 3145-3157.	3.2	6
89	Partially folded states of HIV-1 protease: Molecular dynamics simulations and ligand binding. Computational and Theoretical Chemistry, 2006, 769, 111-121.	1.5	6
90	Computational prediction of selectivities in nonreversible and reversible hydroformylation reactions catalyzed by unmodified rhodium-carbonyls. Journal of Molecular Modeling, 2011, 17, 2275-2284.	1.8	6

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91	High linear regioselectivity in the rhodium-catalyzed hydro(deuterio)formylation of 3,4,4-trimethylpent-1-ene: The role of Î²-hydride elimination. Journal of Molecular Catalysis A, 2012, 356, 1-13.	4.8	6
92	Basis set validation for polyatomic cation-water interactions. Molecular Engineering, 1992, 2, 137-152.	0.2	5
93	Stepwise versus concerted mechanisms in the Wittig reaction in vacuo and in THF: the case of 2,4-dimethyl-3-pyrrol-1-yl-pentanal and triphenylphosphonium ylide. Theoretical Chemistry Accounts, 2009, 123, 337-346.	1.4	5
94	Theoretical study of the stability of myrsinone in vacuo and in solution. Theoretical Chemistry Accounts, 2000, 104, 210-217.	1.4	4
95	Rhodium-Catalyzed Hydroformylation of Ketal-Masked Î²-Isophorone: Computational Explanation for the Unexpected Reaction Evolution of the Tertiary Rh-Alkyl via an Exocyclic Î²-Elimination Derivative. Journal of Physical Chemistry A, 2015, 119, 5117-5133.	2.5	3
96	N-allylpyrrole as a bifunctional precursor to electrically conducting and filmable organic polymers: synthesis and preliminary characterization. Synthetic Metals, 1994, 67, 235-239.	3.9	2
97	Stability of a constrained peptide-based antagonist of neurokinin A, as described by ab initio, semiempirical and empirical calculations. Computational and Theoretical Chemistry, 1998, 426, 339-347.	1.5	2
98	Transferable group contributions for a variety of chemical phenomena and compounds. Theoretical Chemistry Accounts, 2003, 110, 446-459.	1.4	2
99	Is the bias introduced in a FEP calculation by parameterizing a QM reaction acceptable? Comparison with Carâ€“Parrinello MD/AMBER results for the second proton transfer in triosephosphate isomerase (TIM). Computational and Theoretical Chemistry, 2005, 729, 131-139.	1.5	2
100	The fate of branched and linear isomers in the rhodium-catalyzed hydroformylation of 3,4,4-trimethylpent-1-ene. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	2
101	Computational Approaches to the Study of Protein â€" Ligand Interactions. , 1987, , 13-28.		2
102	Graphical description on the solute surface of the solvation energy and solvent transfer energy. Journal of Molecular Graphics, 1989, 7, 170-171.	1.1	1
103	Reaction mechanisms between methylamine and a few Schiff bases: Ab initio potential energy surfaces of a catalytic step in semicarbazide sensitive amino oxidases (SSAO). International Journal of Quantum Chemistry, 2001, 84, 740-749.	2.0	1
104	A test case for time-dependent density functional theory calculations of electronic circular dichroism: 2-chloro-4-methoxy-6- [(R)-1-phenylethylamino]-1,3,5- triazine. Theoretical Chemistry Accounts, 2007, 117, 793-803.	1.4	1
105	Free energy landscapes in THF for the wittig reaction of acetaldehyde and triphenylphosphonium ylide. International Journal of Quantum Chemistry, 2010, 110, 2509-2521.	2.0	1
106	Theoretical study in vacuo of the first step of the reversible aldol cleavage catalyzed by aldolase from rabbit muscle. Computational and Theoretical Chemistry, 1993, 287, 253-259.	1.5	0
107	The fate of branched and linear isomers in the rhodium-catalyzed hydroformylation of 3,4,4-trimethylpent-1-ene. Highlights in Theoretical Chemistry, 2013, , 67-86.	0.0	0