Oscar N Ventura

List of Publications by Year
in descending order

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114 papers	1,876 citations	279798 23 h-index	330143 37 g-index
139 all docs	139 docs citations	139 times ranked	1759 citing authors

#	Article	IF	Citations
1	Electronic and Structural Distortions in Graphene Induced by Carbon Vacancies and Boron Doping. Journal of Physical Chemistry C, 2010, 114, 18961-18971.	3.1	148
2	Acidity of hydroxamic acids: an ab initio and semiempirical study. Journal of the American Chemical Society, 1993, 115, 5754-5761.	13.7	82
3	Quantum model of catalysis based on a mobile proton revealed by subatomic x-ray and neutron diffraction studies of h-aldose reductase. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 1844-1848.	7.1	74
4	Tautomeric Forms of 2-Thiobarbituric Acid As Studied in the Solid, in Polar Solutions, and on Gold Nanoparticles. Journal of Physical Chemistry C, 2007, 111, 3369-3383.	3.1	59
5	Theoretical study of reaction mechanisms for the ketonization of vinyl alcohol in gas phase and aqueous solution. Theoretica Chimica Acta, 1987, 72, 175-195.	0.8	56
6	Density functional study of technetium and rhenium compounds. Computational and Theoretical Chemistry, 2002, 580, 107-116.	1.5	56
7	The FO2 radical: a new success of density functional theory. Chemical Physics Letters, 1995, 245, 488-497.	2.6	50
8	Gas-Phase Structure and Acidity of Formohydroxamic Acid and Formamide: A Comparative ab Initio Study. The Journal of Physical Chemistry, 1995, 99, 131-136.	2.9	49
9	Density functional investigation of atmospheric sulfur chemistry. I. Enthalpy of formation of HSO and related molecules. International Journal of Quantum Chemistry, 2000, 80, 439-453.	2.0	44
10	Theoretical study of the addition of hydrogen halides to olefins: reaction of dimeric hydrogen fluoride with ethylene. Journal of the American Chemical Society, 1986, 108, 923-928.	13.7	42
11	AM1 study of hydrogen bonded complexes of water. Computational and Theoretical Chemistry, 1989, 187, 55-68.	1.5	42
12	Analysis of the gas-phase addition of water to formaldehyde: A semiempirical andab initiostudy of bifunctional catalysis by H2O. Journal of Computational Chemistry, 1992, 13, 1037-1046.	3.3	42
13	Complete basis set and density functional determination of the enthalpy of formation of the controversial HO3 radical: a discrepancy between theory and experiment. Chemical Physics Letters, 2002, 365, 440-449.	2.6	39
14	Theoretical studies of hydrogen-bonded complexes using semiempirical methods. Computational and Theoretical Chemistry, 1990, 210, 405-426.	1.5	36
15	Importance of water in aldol condensation reactions of acetaldehyde. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1745-1755.	1.7	34
16	Density functional investigations of carboxyl free radicals: Formyloxyl, acetyloxyl, and benzoyloxyl radicals. International Journal of Quantum Chemistry, 1998, 70, 253-267.	2.0	34
17	Molecular orbital study of the structures of hydroxamic acids. The Journal of Physical Chemistry, 1992, 96, 3709-3712.	2.9	32
18	Density Functional Theory Is More Accurate Than Coupled-Cluster Theory in the Study of the Thermochemistry of Species Containing the Fâ˜’O Bond. Journal of Physical Chemistry A, 1999, 103, 147-151.	2.5	32

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19	Density functional investigation of atmospheric sulfur chemistry II. The heat of formation of the XSO2 radicals X=H,CH3. Chemical Physics Letters, 2001, 344, 221-228.	2.6	31
20	Density functional study of the decomposition pathways of nitroethane and 2-nitropropaneElectronic supplementary information (ESI) available: The structure of minima on the PES of nitroethane (Fig. S1) and 2-nitropropane (Fig. S2). See http://www.rsc.org/suppdata/cp/b3/b300275f/. Physical Chemistry Chemical Physics, 2003, 5, 1730-1738.	2.8	31
21	A discrepancy between experimental and theoretical thermochemical characterization of some oxygen fluorides. Chemical Physics Letters, 1998, 287, 597-600.	2.6	28
22	Theoretical study of the addition of hydrogen halides to olefins: A comparison between (HCl)2and (HF)2additions to ethylene. Journal of Computational Chemistry, 1987, 8, 481-488.	3.3	27
23	Synthesis, structure and magnetic properties of Mn(II) and Cu(II) complexes with the dicyano-acetic acid methyl ester anion. Inorganica Chimica Acta, 2001, 314, 83-90.	2.4	24
24	Hydroxamic chelates of boric acid, a density functional study. Computational and Theoretical Chemistry, 2001, 537, 173-180.	1.5	23
25	Ab Initio and Density Functional Study of Thionitroso XNS and Thiazyl Isomers XSN, X = H, F, Cl, Br, OH, SH, NH2, CH3, CF3, and SiF3. Journal of Physical Chemistry A, 2004, 108, 5073-5080.	2.5	23
26	Use of bibliometric information to assist research policy making. A comparison of publication and citation profiles of Full and Associate Professors at a School of Chemistry in Uruguay. Scientometrics, 2006, 69, 287-313.	3.0	23
27	Comparison of semiempirical and bsse corrected mÃ¸ller-plesset ab initio calculations on the direct addition of water to formaldehyde. Computational and Theoretical Chemistry, 1990, 210, 427-440.	1.5	22
28	Ab initio study of the structure and reactivity of H2CO.cntdot.H2O.bul.+ and related radical cations. Journal of the American Chemical Society, 1993, 115, 9121-9126.	13.7	22
29	Equilibrium structure of the carbon dioxide-water complex in the gas phase: an ab initio and density functional study. Computational and Theoretical Chemistry, 1997, 390, 157-167.	1.5	21
30	Density functional and coupled-cluster calculations of isodesmic reactions involving fluorine oxides. Chemical Physics Letters, 1999, 301, 331-335.	2.6	20
31	Water-Chain intervention in the ketonization of vinyl alcohol. An ab initio study. International Journal of Quantum Chemistry, 1986, 30, 467-477.	2.0	19
32	Density functional computational thermochemistry: solving the discrepancy between MO and DFT calculations on the enthalpy of formation of sulfine, CH2Š...SŠ...O. Chemical Physics Letters, 2002, 355, 207-213.	2.6	19
33	A theoretical study of excited state proton transfer in 3-hydroxychromone and related molecules. Computational and Theoretical Chemistry, 1999, 487, 221-230.	1.5	18
34	Reinvestigation of the Deceptively Simple Reaction of Toluene with OH and the Fate of the Benzyl Radical: The â€œHiddenâ€•Routes to Cresols and Benzaldehyde. Journal of Physical Chemistry A, 2020, 124, 5917-5930.	2.5	18
35	SVECV â€ƒ12: Benchmark of a composite scheme for accurate and cost effective evaluation of reaction barriers. International Journal of Quantum Chemistry, 2021, 121, e26745.	2.0	18
36	Density Functional Theory: A Useful Tool for the Study of Free Radicals. Advances in Quantum Chemistry, 1997, , 293-309.	0.8	17

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37	Density functional computational thermochemistry: determination of the enthalpy of formation of sulfine, CH2ĩ…Sĩ…O, at room temperature. Chemical Physics Letters, 2000, 329, 145-153.	2.6	17
38	Density Functional Computational Thermochemistry:Â Isomerization of Sulfine and Its Enthalpy of Formation. Journal of Physical Chemistry A, 2001, 105, 9912-9916.	2.5	17
39	Mechanism of the Organocatalyzed Decarboxylative Knoevenagelâ^'Doebner Reaction. A Theoretical Study. Journal of Physical Chemistry A, 2010, 114, 13086-13092.	2.5	15
40	Density functional and G2 study of the strength of the OH bond in CF3OH. Chemical Physics Letters, 1997, 277, 490-496.	2.6	14
41	Low-Temperature Magnetic Properties of LuBaCuFeO5+Î´ and TmBaCuFeO5+Î´. Journal of Solid State Chemistry, 2002, 166, 251-258.	2.9	14
42	CCSDT study of the fluoroperoxyl radical, FOO. Chemical Physics Letters, 2004, 385, 292-297.	2.6	14
43	Ab initiostudy of substituent effect on the addition of hydrogen fluoride to fluoroethylenes. Journal of Computational Chemistry, 1990, 11, 170-180.	3.3	13
44	Comparative ab initio and semi-empirical study of hydrogen bonded complexes of NH3 and H2O. Computational and Theoretical Chemistry, 1992, 254, 315-328.	1.5	13
45	Multireference configuration interaction calculation of the potential energy curves for Oî—¸H bond breaking in the ground and lowest excited states of the water monomer and dimer. Journal of Molecular Structure, 1993, 297, 337-345.	3.6	12
46	Moments of energy level distributions in vibrational spectra. Journal of Physics A, 1993, 26, 5581-5593.	1.6	12
47	The dimerization shift of the OH-stretching fundamentals of the water dimer. Chemical Physics Letters, 1994, 217, 436-442.	2.6	12
48	Structural and conformational analysis of Tcv and Rev dioxo complexes. X-ray crystal structure of [TcO2(tn)2]Â·H2O. Polyhedron, 1997, 16, 3311-3316.	2.2	12
49	A New Perspective in the Lewis Acid Catalyzed Ring Opening of Epoxides. Theoretical Study of Some Complexes of Methanol, Acetic Acid, Dimethyl Ether, Diethyl Ether, and Ethylene Oxide with Boron Trifluoride. Journal of Physical Chemistry A, 2006, 110, 11734-11751.	2.5	12
50	Isomerization of the formaldehyde radical cation and the failure of MP2. Chemical Physics Letters, 1993, 202, 479-482.	2.6	11
51	Density Functional Computational Thermochemistry:â€‰ Determination of the Enthalpy of Formation of Methanethial-S,S-dioxide (Sulfene). Journal of Physical Chemistry A, 2003, 107, 518-521.	2.5	11
52	Molecular Structure and Internal Rotation in 2,3,5,6-Tetrafluoroanisole as Studied by Gas-Phase Electron Diffraction and Quantum Chemical Calculations. Journal of Physical Chemistry A, 2005, 109, 394-399.	2.5	11
53	Regioselective epoxide ring-opening using boron trifluoride diethyl etherate: DFT study of an alternative mechanism to explain the formation of syn-fluorohydrins. Computational and Theoretical Chemistry, 2009, 904, 21-27.	1.5	11
54	Calculations of the infrared and Raman spectra of simple thiols and thiolâ€“water complexes. International Journal of Quantum Chemistry, 2011, 111, 1843-1857.	2.0	11

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55	Structural insights into human microsomal epoxide hydrolase by combined homology modeling, molecular dynamics simulations, and molecular docking calculations. Proteins: Structure, Function and Bioinformatics, 2017, 85, 720-730.	2.6	11
56	Isomerization and Fragmentation Reactions on the [C₂SH₄] Potential Energy Surface: The Metastable Thione S-Methylide Isomer. Journal of Organic Chemistry, 2021, 86, 2941-2956.	3.2	11
57	T- and pH-Dependent Kinetics of the Reactions of Â·OH_(aq) with Glutaric and Adipic Acid for Atmospheric Aqueous-Phase Chemistry. ACS Earth and Space Chemistry, 2021, 5, 1854-1864.	2.7	11
58	Density functional study of isomerization of fluoro- and chloroformaldehyde radical cations. Journal of Computational Chemistry, 1996, 17, 1309-1317.	3.3	10
59	Density functional and ab initio study of the free radical MgNC. Computational and Theoretical Chemistry, 1998, 422, 133-141.	1.5	10
60	Density functional computational thermochemistry: Accurate determination of the enthalpy of formation of perfluoropropane from DFT and ab initio calculations on isodesmic reactions. Chemical Physics Letters, 2005, 403, 378-384.	2.6	9
61	Unraveling the role of additional OH-radicals in the Hâ€“Abstraction from Dimethyl sulfide using quantum chemical computations. Chemical Physics Letters, 2020, 739, 136963.	2.6	9
62	H-Abstraction from Dimethyl Sulfide in the Presence of an Excess of Hydroxyl Radicals. A Quantum Chemical Evaluation of Thermochemical and Kinetic Parameters Unveils an Alternative Pathway to Dimethyl Sulfoxide. ACS Earth and Space Chemistry, 2020, 4, 403-419.	2.7	9
63	Transition states for hydrogen radical reactions: LiFH as a stringent test case for density functional methods. Molecular Physics, 1996, 89, 1851-1870.	1.7	9
64	Highâ€level ab initio prediction of the structure and infrared spectra of formaldehydeâ€“water radicalâ€cation complexes. Journal of Chemical Physics, 1995, 102, 2833-2840.	3.0	8
65	An analysis of dipole polarizabilities using density functional theory: N2, H2, Fâ^' and HF. Journal of Molecular Structure, 1997, 436-437, 489-501.	3.6	8
66	DYNGA: a general purpose QM-MM-MD program. I. Application to water. Molecular Physics, 2003, 101, 2659-2668.	1.7	8
67	ReO2+chelates with aliphatic diamines. Structural and proton transfer properties. New Journal of Chemistry, 2006, 30, 1650-1654.	2.8	8
68	Density functional and chemical model study of the competition between methyl and hydrogen scission of propane and Î²-scission of the propyl radical. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	8
69	On the application of some solvation models to the water dimer. Theoretica Chimica Acta, 1984, 64, 229-248.	0.8	7
70	Molecular modelling of glutathione: a comparison with crystallographic data. Computational and Theoretical Chemistry, 1990, 210, 467-475.	1.5	7
71	A comparative density functional study of the torsional potential of 4-fluoro (trifluoromethoxy)benzene and related species. Chemical Physics Letters, 2004, 389, 405-412.	2.6	7
72	Improved homology model of cyclohexanone monooxygenase from Acinetobacter calcoaceticus based on multiple templates. Computational Biology and Chemistry, 2014, 49, 14-22.	2.3	7

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73	Ab initio characterization of possible dissociation pathways for multiphoton ionization of the water dimer in supersonic free jets. Computational and Theoretical Chemistry, 1992, 254, 453-463.	1.5	6
74	Ab initio study of the structure of radical cations derived from H-bonded complexes: A comparison between [H2CO Â· H2O]+Â· and [H2CO Â· HF]+Â·. Computational and Theoretical Chemistry, 1994, 314, 31-38.	1.5	6
75	Glycine conformations: gradient-corrected DFT-studies. Computational and Theoretical Chemistry, 1998, 433, 193-201.	1.5	6
76	On the structure, infrared and Raman spectra of the 2:1 cysteineâ€“Zn complex. Theoretical Chemistry Accounts, 2010, 125, 279-291.	1.4	6
77	Theoretical Investigation on the Oligomerization of Methylglyoxal and Glyoxal in Aqueous Atmospheric Aerosol Particles. ACS Earth and Space Chemistry, 0, , .	2.7	6
78	Dipolar 1,3â€cycloaddition of thioformaldehyde S â€methylide (<scp> CH ₂ SCH) Tj ETQq0 0 0 rgBT /Overlock 10 T ₃ </scp> , <scp> SO ₂ </scp> , <scp>. Journal of Computational Chemistry, 2022, 43, 1420-1433.	3.3	6
79	Ab initio MP2, MCSCF and MR-SDCI study on the structure of O4 and comparison with the hypervalent CO3 and SO3 species. Computational and Theoretical Chemistry, 1995, 335, 63-68.	1.5	5
80	In-Silico Nanobio-Design. A New Frontier in Computational Biology. Current Topics in Medicinal Chemistry, 2007, 7, 1537-1540.	2.1	5
81	Theoretical study of the structure of neutral, radical and anionic monoperoxo carbonic acid. Computational and Theoretical Chemistry, 2009, 913, 131-138.	1.5	5
82	Theoretical insight into the mechanism for the inhibition of the cysteine protease cathepsin B by 1,2,4-thiadiazole derivatives. Journal of Molecular Modeling, 2014, 20, 2254.	1.8	5
83	Theoretical study of the microhydration of 1â€chloro and 2â€chloro ethanol as a clue for their relative propensity toward dehalogenation. International Journal of Quantum Chemistry, 2019, 119, e25931.	2.0	5
84	Basis Set Effects in the Description of the Cl-O Bond in ClO and XClO/ClOX Isomers (Xâ€‰=â€‰H, O, and Cl) Using DFT and CCSD(T) Methods. Journal of Chemistry, 2019, 2019, 1-23.	1.9	5
85	A reinvestigation of the deceptively simple reaction of toluene with OH, and the fate of the benzyl radical: a combined thermodynamic and kinetic study on the competition between OH-addition and H-abstraction reactions. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	5
86	T- and pH-dependent OH radical reaction kinetics with glycine, alanine, serine, and threonine in the aqueous phase. Physical Chemistry Chemical Physics, 2022, , .	2.8	5
87	Computational determination of the enthalpy of formation of alkylthial S-oxides and alkylthione S-oxides: a study of (Z)-propanethial-S-oxide, the lachrymatory factor of the onion (Allium cepa). Physical Chemistry Chemical Physics, 2002, 4, 4328-4333.	2.8	3
88	Comparison of large basis set DFT and MP2 calculations in the study of the barrier for internal rotation of 2,3,5,6-tetrafluoroanisole. International Journal of Quantum Chemistry, 2007, 107, 403-417.	2.0	3
89	Conformational analysis of trans-[ReO2(pn)2]+ in aqueous solution by NMR and DFT calculations. Journal of Molecular Structure, 2008, 892, 146-150.	3.6	3
90	On the experimental structure of monoperoxocarbonic acid and the enthalpy of formation of carbonic acid, peroxyformic acid and monoperoxocarbonic acid in gas phase. Chemical Physics Letters, 2009, 480, 52-56.	2.6	3

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91	Interaction of Simple Ions with Water: Theoretical Models for the Study of Ion Hydration. Journal of Chemical Education, 2009, 86, 1403.	2.3	3
92	Computational study on the partial dechlorination of the pesticide chloropicrin by sulfur species. Theoretical Chemistry Accounts, 2011, 130, 955-963.	1.4	3
93	Computational characterization of the herbicide metolachlor and its mono-hydroxylated photodegradation products. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	3
94	Enthalpies of formation of the benzyloxyl, benzylperoxyl, hydroxyphenyl radicals and related species on the potential energy surface for the reaction of toluene with the hydroxyl radical. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	3
95	Thecis-trans energy difference in bi-1-cyclopro-pen-1-yl and related compounds. Theoretica Chimica Acta, 1980, 56, 157-162.	0.8	2
96	A semiempirical study of the reaction of the hemimercaptal of methylglyoxal and glutathione at the active center of glyoxalase I. International Journal of Quantum Chemistry, 1992, 44, 699-722.	2.0	2
97	Dichloro(cyclohexilidene-1-methylene)(phenyl)Te(IV). Looking for the theoretical treatment. Zeitschrift Fur Kristallographie - Crystalline Materials, 2004, 219, 652-658.	0.8	2
98	Computational Evidence Suggests That 1-Chloroethanol May Be an Intermediate in the Thermal Decomposition of 2-Chloroethanol into Acetaldehyde and HCl. Journal of Physical Chemistry A, 2019, 123, 1983-1998.	2.5	2
99	A quatum-mechanical study of metheyl fluoroformate. Chemical Physics Letters, 1980, 70, 170-174.	2.6	1
100	On the structure of the 3B1 excited state of water. Computational and Theoretical Chemistry, 1995, 334, 127-136.	1.5	1
101	EXPERIMENTAL AND THEORETICAL STUDY OF THE MOVEMENT OF THE WPD FLEXIBLE LOOP OF HUMAN PROTEIN TYROSINE PHOSPHATASE PTP1B IN COMPLEX WITH HALIDE IONS. Biophysical Reviews and Letters, 2012, 07, 197-217.	0.8	1
102	Using density functional theory to increase the accuracy of experimental crystal structures: The case of potassium peroxocarbonate. Journal of Molecular Structure, 2017, 1146, 1-4.	3.6	1
103	Tropospheric degradation of propanethiol initiated by Cl radicals: Kinetics, mechanism and computational studies. Chemical Physics Letters, 2019, 723, 69-75.	2.6	1
104	From science-fiction to present life. Physics of Life Reviews, 2020, 32, 121-123.	2.8	1
105	Calculation of the Geometries and Infrared Spectra of the Stacked Cofactor Flavin Adenine Dinucleotide (FAD) as the Prerequisite for Studies of Light-Triggered Proton and Electron Transfer. Biomolecules, 2020, 10, 573.	4.0	1
106	Degradation mechanism of 2-fluoropropene by Cl atoms: experimental and theoretical products distribution studies. Physical Chemistry Chemical Physics, 2022, , .	2.8	1
107	An AM1 semiempirical study of the mechanism of sintering for ZnO in the presence of water and carbon dioxide. Computational and Theoretical Chemistry, 1994, 305, 175-184.	1.5	0
108	Density of levels in vibrational spectra of molecules. International Journal of Quantum Chemistry, 1997, 63, 835-842.	2.0	0

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109	AccuModel vl.1 for Windows 95. Journal of Chemical Information and Computer Sciences, 1998, 38, 768-770.	2.8	0
110	The Quitel-2002. Theoretical Chemistry Accounts, 2003, 110, 359-359.	1.4	0
111	Ab initio and Density Functional Study of Thionitroso XNS and Thiazyl Isomers XSN, X: H, F, Cl, Br, OH, SH, NH2, CH3, CF3, and SiF3.. ChemInform, 2004, 35, no.	0.0	0
112	Theoretical study of the reactions of the hydroselenyl radical (HSeâ—) with the selenenic radical (HSeOâ—). Journal of Molecular Modeling, 2018, 24, 3.	1.8	0
113	Diffusion and reptation quantum Monte Carlo study of the NaK molecule. Molecular Physics, 2019, 117, 813-822.	1.7	0
114	Kinetics and thermodynamics of the hydroxylation products in the photodegradation of the herbicide Metolachlor. Pure and Applied Chemistry, 2020, 92, 473-484.	1.9	0