Ignacio Fdez GalvÃ¡n

List of Publications by Year
in descending order

75 papers	3,996 citations	257101 24 h-index	118652 62 g-index

87 all docs	87 docs citations	87 times ranked	4252 citing authors

#	Article	IF	Citations
1	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	1.5	1,317
2	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661
3	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	1.2	281
4	Chemi- and Bioluminescence of Cyclic Peroxides. Chemical Reviews, 2018, 118, 6927-6974.	23.0	265
5	Analytical State-Average Complete-Active-Space Self-Consistent Field Nonadiabatic Coupling Vectors: Implementation with Density-Fitted Two-Electron Integrals and Application to Conical Intersections. Journal of Chemical Theory and Computation, 2016, 12, 3636-3653.	2.3	112
6	Geometry optimization of molecules in solution: Joint use of the mean field approximation and the free-energy gradient method. Journal of Chemical Physics, 2003, 118, 255-263.	1.2	93
7	ASEP/MD: A program for the calculation of solvent effects combining QM/MM methods and the mean field approximation. Computer Physics Communications, 2003, 155, 244-259.	3.0	85
8	How machine learning can assist the interpretation of ab initio molecular dynamics simulations and conceptual understanding of chemistry. Chemical Science, 2019, 10, 2298-2307.	3.7	80
9	Unraveling factors leading to efficient norbornadieneâ€“quadricyclane molecular solar-thermal energy storage systems. Journal of Materials Chemistry A, 2017, 5, 12369-12378.	5.2	65
10	A QM/MM study of proton transport pathways in a [NiFe] hydrogenase. Proteins: Structure, Function and Bioinformatics, 2008, 73, 195-203.	1.5	58
11	Quantum mechanical methods applied to excitation energy transfer: A comparative analysis on excitation energies and electronic couplings. Journal of Chemical Physics, 2008, 129, 034104.	1.2	54
12	Theoretical Calculation of the Stark Component of the Soluteâ^'Solvent Interaction Energy. Validity of the Mean Field Approximation in the Study of Liquids and Solutions. Journal of Physical Chemistry B, 2002, 106, 4813-4817.	1.2	52
13	A new method to locate saddle points for reactions in solution by using the free-energy gradient method and the mean field approximation. Journal of Computational Chemistry, 2004, 25, 1227-1233.	1.5	40
14	A theoretical study of solvent effects on the 1(nâ†'Ï€*) electron transition in acrolein. Journal of Chemical Physics, 2004, 121, 3710-3716.	1.2	37
15	Mechanism of activated chemiluminescence of cyclic peroxides: 1,2-dioxetanes and 1,2-dioxetanones. Physical Chemistry Chemical Physics, 2017, 19, 3955-3962.	1.3	37
16	Impact of Excited-State Antiaromaticity Relief in a Fundamental Benzene Photoreaction Leading to Substituted Bicyclo[3.1.0]hexenes. Journal of the American Chemical Society, 2020, 142, 10942-10954.	6.6	37
17	Theoretical Study of the Dual Fluorescence of 4-(N,N-Dimethylamino)benzonitrile in Solution. Journal of Chemical Theory and Computation, 2010, 6, 2445-2454.	2.3	35
18	A CASPT2//CASSCF Study of Vertical and Adiabatic Electron Transitions of Acrolein in Water Solution. Journal of Physical Chemistry B, 2007, 111, 9864-9870.	1.2	34

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19	Improving the efficiency of the NEB reaction path finding algorithm. Journal of Computational Chemistry, 2008, 29, 139-143.	1.5	30
20	Restricted-Variance Molecular Geometry Optimization Based on Gradient-Enhanced Kriging. Journal of Chemical Theory and Computation, 2020, 16, 3989-4001.	2.3	28
21	Study on the conformational equilibrium of the alanine dipeptide in water solution by using the averaged solvent electrostatic potential from molecular dynamics methodology. Journal of Chemical Physics, 2011, 135, 194502.	1.2	26
22	Solvent Effects on the Radiative and Nonradiative Decay of a Model of the Rhodopsin Chromophore. Journal of Chemical Theory and Computation, 2011, 7, 4050-4059.	2.3	26
23	Dynamical Insights into the Decomposition of 1,2-Dioxetane. Journal of Chemical Theory and Computation, 2017, 13, 2448-2457.	2.3	25
24	Solvent Effects on the Low-Lying Excited States of a Model of Retinal. Journal of Physical Chemistry B, 2006, 110, 18064-18071.	1.2	24
25	Theoretical Study of the Preferential Solvation Effect on the Solvatochromic Shifts of para-Nitroaniline. Journal of Physical Chemistry B, 2013, 117, 2466-2474.	1.2	24
26	Optomechanical Control of Quantum Yield in Transâ€“Cis Ultrafast Photoisomerization of a Retinal Chromophore Model. Angewandte Chemie - International Edition, 2017, 56, 3842-3846.	7.2	24
27	How Do Methyl Groups Enhance the Triplet Chemiexcitation Yield of Dioxetane?. Journal of Physical Chemistry Letters, 2017, 8, 3790-3794.	2.1	24
28	Location of conical intersections in solution using a sequential quantum mechanics/molecular dynamics method. Chemical Physics Letters, 2007, 443, 76-81.	1.2	20
29	Restricted-Variance Constrained, Reaction Path, and Transition State Molecular Optimizations Using Gradient-Enhanced Kriging. Journal of Chemical Theory and Computation, 2021, 17, 571-582.	2.3	20
30	Theoretical Study of Solvent Effects on the Ground and Low-Lying Excited Free Energy Surfaces of a Pushâ€“Pull Substituted Azobenzene. Journal of Physical Chemistry B, 2014, 118, 12518-12530.	1.2	18
31	On the absorption properties of the excited states of DMABN. Chemical Physics Letters, 2010, 499, 100-102.	1.2	17
32	Theoretical Study of the 1,3-Hydrogen Shift of Triazene in Water. Journal of Physical Chemistry B, 2005, 109, 23024-23030.	1.2	16
33	Retinal Models: Comparison of Electronic Absorption Spectra in the Gas Phase and in Methanol Solution. Journal of Physical Chemistry B, 2008, 112, 8815-8823.	1.2	16
34	Solvatochromic Shifts on Absorption and Fluorescence Bands of N,N-Dimethylaniline. Journal of Chemical Theory and Computation, 2009, 5, 341-349.	2.3	16
35	Theoretical Study of Liquid Hydrogen Fluoride. Application of the Averaged Solvent Electrostatic Potential/Molecular Dynamics Method. Journal of Physical Chemistry B, 2003, 107, 5043-5047.	1.2	15
36	Optomechanical Control of Quantum Yield in Transâ€“Cis Ultrafast Photoisomerization of a Retinal Chromophore Model. Angewandte Chemie, 2017, 129, 3900-3904.	1.6	15

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37	Solvent Effects on the Structure and Spectroscopy of the Emitting States of 1-Phenylpyrrole. Journal of Chemical Theory and Computation, 2011, 7, 1850-1857.	2.3	14
38	Simultaneous Solvent and Counterion Effects on the Absorption Properties of a Model of the Rhodopsin Chromophore. Journal of Chemical Theory and Computation, 2013, 9, 1548-1556.	2.3	14
39	Substituent and Solvent Effects on the UVâ€“vis Absorption Spectrum of the Photoactive Yellow Protein Chromophore. Journal of Physical Chemistry A, 2015, 119, 5504-5514.	1.1	13
40	Solvent Effects on Internal Conversions and Intersystem Crossings:Â The Radiationless De-Excitation of Acrolein in Water. Journal of Physical Chemistry B, 2008, 112, 877-884.	1.2	12
41	Solvent Effects on the Absorption Spectra of the para-Coumaric Acid Chromophore in Its Different Protonation Forms. Journal of Chemical Theory and Computation, 2013, 9, 4481-4494.	2.3	12
42	A combined theoretical and experimental study on the mechanism of spiro-adamantyl-1,2-dioxetanone decomposition. RSC Advances, 2017, 7, 17462-17472.	1.7	12
43	Role of conical intersection seam topography in the chemiexcitation of 1,2-dioxetanes. Physical Chemistry Chemical Physics, 2022, 24, 1638-1653.	1.3	12
44	Theoretical Study of the Competition between Intramolecular Hydrogen Bonds and Solvation in the Cys-Asn-Ser Tripeptide. Journal of Physical Chemistry B, 2010, 114, 8961-8970.	1.2	11
45	Inner projection techniques for the low-cost handling of two-electron integrals in quantum chemistry. Molecular Physics, 2017, 115, 2052-2064.	0.8	11
46	An averaged solvent electrostatic potential from molecular dynamics study of the anomeric equilibrium of D-xylose in aqueous solution. Theoretical Chemistry Accounts, 2004, 111, 196-203.	0.5	10
47	Framework-based design of a new all-purpose molecular simulation application: The Adun simulator. Journal of Computational Chemistry, 2005, 26, 1647-1659.	1.5	10
48	Comparison of three effective Hamiltonian models of increasing complexity: Triazene in water as a test case. Journal of Chemical Physics, 2006, 124, 214504.	1.2	10
49	Theoretical study of the role of solvent Stark effect in electron transitions. Theoretical Chemistry Accounts, 2011, 128, 783-793.	0.5	10
50	Theoretical study of the conformational equilibrium of 1,4-dioxane in gas phase, neat liquid, and dilute aqueous solutions. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	10
51	An ASEP/MD study of liquid chloroform. Computational and Theoretical Chemistry, 2006, 775, 81-86.	1.5	9
52	QM/MM Study of Substituent and Solvent Effects on the Excited State Dynamics of the Photoactive Yellow Protein Chromophore. Journal of Chemical Theory and Computation, 2017, 13, 737-748.	2.3	8
53	Triplet versus singlet chemiexcitation mechanism in dioxetanone: a CASSCF/CASPT2 study. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	8
54	Competition between ring-puckering and ring-opening excited state reactions exemplified on 5H-furan-2-one and derivatives. Journal of Chemical Physics, 2020, 152, 064301.	1.2	8

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55	Beyond the Continuum Approach. , 0, , 499-605.		6
56	Spectroscopy of linear and circular polarized light with the exact semiclassical lightâ€“matter interaction. Annual Reports in Computational Chemistry, 2019, 15, 39-76.	0.9	6
57	Machine learning for analysing ab initio molecular dynamics simulations. Journal of Physics: Conference Series, 2020, 1412, 042003.	0.3	6
58	Constrained numerical gradients and composite gradients: Practical tools for geometry optimization and potential energy surface navigation. Journal of Computational Chemistry, 2015, 36, 1698-1708.	1.5	5
59	Exact semi-classical lightâ€“matter interaction operator applied to two-photon processes with strong relativistic effects. Journal of Chemical Physics, 2020, 153, 024114.	1.2	5
60	The Enamine Intermediate May Not Be Universal to Thiamine Catalysis. Angewandte Chemie - International Edition, 2007, 46, 9019-9022.	7.2	4
61	Chemiexcitation without the Peroxide Bond? Replacing Oxygen with other Heteroatoms. ChemPhotoChem, 2019, 3, 957-967.	1.5	4
62	Advances in computational photochemistry and chemiluminescence of biological and nanotechnological molecules. Photochemistry, 2016, , 16-60.	0.2	4
63	An averaged solvent electrostatic potential/molecular dynamics study of the influence of the electron correlation on the properties of liquid hydrogen fluoride. Computational and Theoretical Chemistry, 2003, 632, 227-234.	1.5	3
64	Dual Fluorescence of Fluorazene in Solution: A Computational Study. Journal of Chemical Theory and Computation, 2011, 7, 3694-3701.	2.3	3
65	Chapter 2. Recent method developments and applications in computational photochemistry, chemiluminescene and bioluminescence. Photochemistry, 2014, , 11-42.	0.2	3
66	Uncontracted basis sets for ab initio calculations of muonic atoms and molecules. International Journal of Quantum Chemistry, 2018, 118, e25755.	1.0	3
67	Photophysical characterization and fluorescence cell imaging applications of 4-N-substituted benzothiadiazoles. RSC Advances, 2022, 12, 14544-14550.	1.7	3
68	Use of the Average Solvent Potential Approach in the Study of Solvent Effects. Advances in Quantum Chemistry, 2010, 59, 59-97.	0.4	2
69	A new QM/MM method oriented to the study of ionic liquids. Journal of Computational Chemistry, 2015, 36, 1893-1901.	1.5	2
70	Non-radiative decay and fragmentation in water molecules after 1a1â^'14a1 excitation and core ionization studied by electron-energy-resolved electronâ€“ion coincidence spectroscopy. Journal of Chemical Physics, 2020, 152, 074302.	1.2	2
71	S₀â†' S₃transition in recombination products of photodissociated dihalomethanes. Molecular Physics, 2014, 112, 575-582.	0.8	1
72	A theoretical analysis of the intrinsic light-harvesting properties of xanthopterin. Computational and Theoretical Chemistry, 2014, 1040-1041, 230-236.	1.1	1

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73	Molecular and Electronic Structure of Re2Br4(PMe3)4. Inorganic Chemistry, 2016, 55, 7111-7116.	1.9	1
74	Solvent Effects on Radiative and Non-Radiative Excited State Decays. Challenges and Advances in Computational Chemistry and Physics, 2008, , 135-157.	0.6	0
75	Accelerating QM/MM Calculations by Using the Mean Field Approximation. Challenges and Advances in Computational Chemistry and Physics, 2015, , 135-152.	0.6	0