

# Ignacio Fdez GalvÃ¡n

## List of Publications by Year in descending order

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75  
papers

3,996  
citations

257450

24  
h-index

118850

62  
g-index

87  
all docs

87  
docs citations

87  
times ranked

4252  
citing authors

#	ARTICLE	IF	CITATIONS
1	<sc>Molcas</sc> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. <i>Journal of Computational Chemistry</i> , 2016, 37, 506-541.	3.3	1,317
2	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5925-5964.	5.3	661
3	Modern quantum chemistry with [Open]Molcas. <i>Journal of Chemical Physics</i> , 2020, 152, 214117.	3.0	281
4	Chemi- and Bioluminescence of Cyclic Peroxides. <i>Chemical Reviews</i> , 2018, 118, 6927-6974.	47.7	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. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3636-3653.	5.3	112
6	Geometry optimization of molecules in solution: Joint use of the mean field approximation and the free-energy gradient method. <i>Journal of Chemical Physics</i> , 2003, 118, 255-263.	3.0	93
7	ASEP/MD: A program for the calculation of solvent effects combining QM/MM methods and the mean field approximation. <i>Computer Physics Communications</i> , 2003, 155, 244-259.	7.5	85
8	How machine learning can assist the interpretation of <i>ab initio</i> molecular dynamics simulations and conceptual understanding of chemistry. <i>Chemical Science</i> , 2019, 10, 2298-2307.	7.4	80
9	Unraveling factors leading to efficient norbornadiene-quadricyclane molecular solar-thermal energy storage systems. <i>Journal of Materials Chemistry A</i> , 2017, 5, 12369-12378.	10.3	65
10	A QM/MM study of proton transport pathways in a [NiFe] hydrogenase. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 73, 195-203.	2.6	58
11	Quantum mechanical methods applied to excitation energy transfer: A comparative analysis on excitation energies and electronic couplings. <i>Journal of Chemical Physics</i> , 2008, 129, 034104.	3.0	54
12	Theoretical Calculation of the Stark Component of the Solute-Solvent Interaction Energy. Validity of the Mean Field Approximation in the Study of Liquids and Solutions. <i>Journal of Physical Chemistry B</i> , 2002, 106, 4813-4817.	2.6	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. <i>Journal of Computational Chemistry</i> , 2004, 25, 1227-1233.	3.3	40
14	A theoretical study of solvent effects on the $1(n\pi^*)$ electron transition in acrolein. <i>Journal of Chemical Physics</i> , 2004, 121, 3710-3716.	3.0	37
15	Mechanism of activated chemiluminescence of cyclic peroxides: 1,2-dioxetanes and 1,2-dioxetanones. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3955-3962.	2.8	37
16	Impact of Excited-State Antiaromaticity Relief in a Fundamental Benzene Photoreaction Leading to Substituted Bicyclo[3.1.0]hexenes. <i>Journal of the American Chemical Society</i> , 2020, 142, 10942-10954.	13.7	37
17	Theoretical Study of the Dual Fluorescence of 4-(N,N-Dimethylamino)benzonitrile in Solution. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2445-2454.	5.3	35
18	A CASPT2//CASSCF Study of Vertical and Adiabatic Electron Transitions of Acrolein in Water Solution. <i>Journal of Physical Chemistry B</i> , 2007, 111, 9864-9870.	2.6	34

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19	Improving the efficiency of the NEB reaction path finding algorithm. <i>Journal of Computational Chemistry</i> , 2008, 29, 139-143.	3.3	30
20	Restricted-Variance Molecular Geometry Optimization Based on Gradient-Enhanced Kriging. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3989-4001.	5.3	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. <i>Journal of Chemical Physics</i> , 2011, 135, 194502.	3.0	26
22	Solvent Effects on the Radiative and Nonradiative Decay of a Model of the Rhodopsin Chromophore. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 4050-4059.	5.3	26
23	Dynamical Insights into the Decomposition of 1,2-Dioxetane. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2448-2457.	5.3	25
24	Solvent Effects on the Low-Lying Excited States of a Model of Retinal. <i>Journal of Physical Chemistry B</i> , 2006, 110, 18064-18071.	2.6	24
25	Theoretical Study of the Preferential Solvation Effect on the Solvatochromic Shifts of <i>para</i> -Nitroaniline. <i>Journal of Physical Chemistry B</i> , 2013, 117, 2466-2474.	2.6	24
26	Optomechanical Control of Quantum Yield in <i>Trans</i> $\leftrightarrow$ <i>Cis</i> Ultrafast Photoisomerization of a Retinal Chromophore Model. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 3842-3846.	13.8	24
27	How Do Methyl Groups Enhance the Triplet Chemiexcitation Yield of Dioxetane?. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3790-3794.	4.6	24
28	Location of conical intersections in solution using a sequential quantum mechanics/molecular dynamics method. <i>Chemical Physics Letters</i> , 2007, 443, 76-81.	2.6	20
29	Restricted-Variance Constrained, Reaction Path, and Transition State Molecular Optimizations Using Gradient-Enhanced Kriging. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 571-582.	5.3	20
30	Theoretical Study of Solvent Effects on the Ground and Low-Lying Excited Free Energy Surfaces of a Push-Pull Substituted Azobenzene. <i>Journal of Physical Chemistry B</i> , 2014, 118, 12518-12530.	2.6	18
31	On the absorption properties of the excited states of DMABN. <i>Chemical Physics Letters</i> , 2010, 499, 100-102.	2.6	17
32	Theoretical Study of the 1,3-Hydrogen Shift of Triazene in Water. <i>Journal of Physical Chemistry B</i> , 2005, 109, 23024-23030.	2.6	16
33	Retinal Models: Comparison of Electronic Absorption Spectra in the Gas Phase and in Methanol Solution. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8815-8823.	2.6	16
34	Solvatochromic Shifts on Absorption and Fluorescence Bands of <i>N,N</i> -Dimethylaniline. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 341-349.	5.3	16
35	Theoretical Study of Liquid Hydrogen Fluoride. Application of the Averaged Solvent Electrostatic Potential/Molecular Dynamics Method. <i>Journal of Physical Chemistry B</i> , 2003, 107, 5043-5047.	2.6	15
36	Optomechanical Control of Quantum Yield in <i>Trans</i> $\leftrightarrow$ <i>Cis</i> Ultrafast Photoisomerization of a Retinal Chromophore Model. <i>Angewandte Chemie</i> , 2017, 129, 3900-3904.	2.0	15

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37	Solvent Effects on the Structure and Spectroscopy of the Emitting States of 1-Phenylpyrrole. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1850-1857.	5.3	14
38	Simultaneous Solvent and Counterion Effects on the Absorption Properties of a Model of the Rhodopsin Chromophore. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1548-1556.	5.3	14
39	Substituent and Solvent Effects on the UV-vis Absorption Spectrum of the Photoactive Yellow Protein Chromophore. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5504-5514.	2.5	13
40	Solvent Effects on Internal Conversions and Intersystem Crossings: The Radiationless De-Excitation of Acrolein in Water. <i>Journal of Physical Chemistry B</i> , 2008, 112, 877-884.	2.6	12
41	Solvent Effects on the Absorption Spectra of the <i>para</i> -Coumaric Acid Chromophore in Its Different Protonation Forms. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4481-4494.	5.3	12
42	A combined theoretical and experimental study on the mechanism of spiro-adamantyl-1,2-dioxetanone decomposition. <i>RSC Advances</i> , 2017, 7, 17462-17472.	3.6	12
43	Role of conical intersection seam topography in the chemiexcitation of 1,2-dioxetanes. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1638-1653.	2.8	12
44	Theoretical Study of the Competition between Intramolecular Hydrogen Bonds and Solvation in the Cys-Asn-Ser Tripeptide. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8961-8970.	2.6	11
45	Inner projection techniques for the low-cost handling of two-electron integrals in quantum chemistry. <i>Molecular Physics</i> , 2017, 115, 2052-2064.	1.7	11
46	An averaged solvent electrostatic potential from molecular dynamics study of the anomeric equilibrium of D-xylose in aqueous solution. <i>Theoretical Chemistry Accounts</i> , 2004, 111, 196-203.	1.4	10
47	Framework-based design of a new all-purpose molecular simulation application: The Adun simulator. <i>Journal of Computational Chemistry</i> , 2005, 26, 1647-1659.	3.3	10
48	Comparison of three effective Hamiltonian models of increasing complexity: Triazene in water as a test case. <i>Journal of Chemical Physics</i> , 2006, 124, 214504.	3.0	10
49	Theoretical study of the role of solvent Stark effect in electron transitions. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 783-793.	1.4	10
50	Theoretical study of the conformational equilibrium of 1,4-dioxane in gas phase, neat liquid, and dilute aqueous solutions. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	1.4	10
51	An ASEP/MD study of liquid chloroform. <i>Computational and Theoretical Chemistry</i> , 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. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 737-748.	5.3	8
53	Triplet versus singlet chemiexcitation mechanism in dioxetanone: a CASSCF/CASPT2 study. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	1.4	8
54	Competition between ring-puckering and ring-opening excited state reactions exemplified on 5H-furan-2-one and derivatives. <i>Journal of Chemical Physics</i> , 2020, 152, 064301.	3.0	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 light-matter interaction. Annual Reports in Computational Chemistry, 2019, 15, 39-76.	1.7	6
57	Machine learning for analysing ab initio molecular dynamics simulations. Journal of Physics: Conference Series, 2020, 1412, 042003.	0.4	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.	3.3	5
59	Exact semi-classical light-matter interaction operator applied to two-photon processes with strong relativistic effects. Journal of Chemical Physics, 2020, 153, 024114.	3.0	5
60	The Enamine Intermediate May Not Be Universal to Thiamine Catalysis. Angewandte Chemie - International Edition, 2007, 46, 9019-9022.	13.8	4
61	Chemexcitation without the Peroxide Bond? Replacing Oxygen with other Heteroatoms. ChemPhotoChem, 2019, 3, 957-967.	3.0	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.	5.3	3
65	Chapter 2. Recent method developments and applications in computational photochemistry, chemiluminescence 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.	2.0	3
67	Photophysical characterization and fluorescence cell imaging applications of 4-N-substituted benzothiadiazoles. RSC Advances, 2022, 12, 14544-14550.	3.6	3
68	Use of the Average Solvent Potential Approach in the Study of Solvent Effects. Advances in Quantum Chemistry, 2010, 59, 59-97.	0.8	2
69	A new QM/MM method oriented to the study of ionic liquids. Journal of Computational Chemistry, 2015, 36, 1893-1901.	3.3	2
70	Non-radiative decay and fragmentation in water molecules after 1a1 <sup>~</sup> 14a1 excitation and core ionization studied by electron-energy-resolved electron-ion coincidence spectroscopy. Journal of Chemical Physics, 2020, 152, 074302.	3.0	2
71	S <sub>0</sub> S <sub>3</sub> transition in recombination products of photodissociated dihalomethanes. Molecular Physics, 2014, 112, 575-582.	1.7	1
72	A theoretical analysis of the intrinsic light-harvesting properties of xanthopterin. Computational and Theoretical Chemistry, 2014, 1040-1041, 230-236.	2.5	1

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73	Molecular and Electronic Structure of $\text{Re}_2\text{Br}_4(\text{PMe}_3)_4$ . <i>Inorganic Chemistry</i> , 2016, 55, 7111-7116.	4.0	1
74	Solvent Effects on Radiative and Non-Radiative Excited State Decays. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2008, , 135-157.	0.6	0
75	Accelerating QM/MM Calculations by Using the Mean Field Approximation. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015, , 135-152.	0.6	0