JosÃ© A GascÃ³n

List of Publications by Year
in descending order

69 papers	2,806 citations	236925 25 h-index	175258 52 g-index
73 all docs	73 docs citations	73 times ranked	2735 citing authors

#	Article	IF	Citations
1	Electronic energy levels of porphyrins are influenced by the local chemical environment. RSC Advances, 2022, 12, 1361-1365.	3.6	4
2	A favorable path to domain separation in the orange carotenoid protein. Protein Science, 2022, 31, 850-863.	7.6	3
3	Interexciton nonradiative relaxation pathways in the peridinin-chlorophyll protein. Cell Reports Physical Science, 2021, 2, 100380.	5.6	7
4	Spectral Features of Canthaxanthin in HCP2. A QM/MM Approach. Molecules, 2021, 26, 2441.	3.8	2
5	Insights into diastereotopic effects in thiolated gold nanoclusters. Chemical Physics Letters, 2021, 770, 138448.	2.6	1
6	High-Throughput Non-targeted Chemical Structure Identification Using Gas-Phase Infrared Spectra. Analytical Chemistry, 2021, 93, 10688-10696.	6.5	4
7	Easily accessible non-aromatic heterocycles with handles: 4-bromo-2,3-dihydrofurans from 1,2-dibromohomoallylic alcohols. Chemical Science, 2021, 12, 10347-10353.	7.4	2
8	Aluminosilicate Mineralogy and the Sorption of Organic Cations: Interplay between Electrostatic Barriers and Compound Structural Features. Environmental Science & Technology, 2020, 54, 1623-1633.	10.0	6
9	Protein polarization effects in the thermodynamic computation of vibrational Stark shifts. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	6
10	Spectral Signatures of Canthaxanthin Translocation in the Orange Carotenoid Protein. Journal of Physical Chemistry B, 2020, 124, 11387-11395.	2.6	12
11	Amide-Linked C4â€³-Saccharide Modification of KRN7000 Provides Potent Stimulation of Human Invariant NKT Cells and Anti-Tumor Immunity in a Humanized Mouse Model. ACS Chemical Biology, 2020, 15, 3176-3186.	3.4	6
12	Fluorescence Anisotropy Detection of Barrier Crossing and Ultrafast Conformational Dynamics in the S₂ State of Î²-Carotene. Journal of Physical Chemistry B, 2020, 124, 9029-9046.	2.6	10
13	Origins of the Electronic Modulations of Bacterio- and Isobacteriodilactone Regioisomers. Journal of Physical Chemistry A, 2019, 123, 7470-7485.	2.5	14
14	Bacterio- and Isobacteriodilactones by Stepwise or Direct Oxidations of meso-Tetrakis(pentafluorophenyl)porphyrin. Journal of Organic Chemistry, 2019, 84, 239-256.	3.2	23
15	Formation of and Glycosylation with Perâ€Oâ€Acetyl Septanosyl Halides: Rationalizing Complex Reactivity En Route to pâ€Nitrophenyl Septanosides. European Journal of Organic Chemistry, 2018, 2018, 1709-1719.	2.4	6
16	Light Harvesting by Equally Contributing Mechanisms in a Photosynthetic Antenna Protein. Journal of Physical Chemistry Letters, 2018, 9, 563-568.	4.6	8
17	Dual Modifications of Î±-Galactosylceramide Synergize to Promote Activation of Human Invariant Natural Killer T Cells and Stimulate Anti-tumor Immunity. Cell Chemical Biology, 2018, 25, 571-584.e8.	5.2	27
18	Atomically precise Au₁₄₄(SR)₆₀ nanoclusters (R = Et, Pr) are capped by 12 distinct ligand types of 5-fold equivalence and display gigantic diastereotopic effects. Chemical Science, 2018, 9, 8796-8805.	7.4	30

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19	Carotenoid-Chlorophyll Interactions in a Photosynthetic Antenna Protein: A Supramolecular QM/MM Approach. Molecules, 2018, 23, 2589.	3.8	7
20	The limited extent of the electronic modulation of chlorins and bacteriochlorins through chromene-annulation. Physical Chemistry Chemical Physics, 2018, 20, 18233-18240.	2.8	4
21	Bacteriochlorins with a Twist: Discovery of a Unique Mechanism to Red-Shift the Optical Spectra of Bacteriochlorins. Journal of the American Chemical Society, 2017, 139, 548-560.	13.7	32
22	Preparation of Some Homologous TEMPO Nitroxides and Oxoammonium Salts; Notes on the NMR Spectroscopy of Nitroxide Free Radicals; Observed Radical Nature of Oxoammonium Salt Solutions Containing Trace Amounts of Corresponding Nitroxides in an Equilibrium Relationship. Journal of Organic Chemistry, 2017, 82, 9279-9290.	3.2	19
23	The MOD-QM/MM Method. Methods in Enzymology, 2016, 577, 443-481.	1.0	4
24	Vibrational Coupling Modulation in n-Alkanethiolate Protected Au₂₅(SR)₁₈⁰ Clusters. Journal of Physical Chemistry C, 2016, 120, 25378-25386.	3.1	20
25	Chromene-Annulated Bacteriochlorins. Journal of Organic Chemistry, 2016, 81, 3603-3618.	3.2	18
26	Fullerene-Assisted Photoinduced Charge Transfer of Single-Walled Carbon Nanotubes through a Flavin Helix. Journal of the American Chemical Society, 2016, 138, 5904-5915.	13.7	15
27	A magnetic look into the protecting layer of Au₂₅ clusters. Chemical Science, 2016, 7, 6910-6918.	7.4	33
28	Connectivity-Based Biocompatible Force Field for Thiolated Gold Nanoclusters. Journal of Physical Chemistry C, 2015, 119, 27804-27812.	3.1	10
29	Interaction of H₂@C₆₀ and Nitroxide through Conformationally Constrained Peptide Bridges. Photochemistry and Photobiology, 2014, 90, 439-447.	2.5	3
30	MoD-QM/MM Structural Refinement Method: Characterization of Hydrogen Bonding in the Oxytricha nova G-Quadruplex. Journal of Chemical Theory and Computation, 2014, 10, 5125-5135.	5.3	16
31	Au₂₅(SEt)₁₈, a Nearly Naked Thiolate-Protected Au₂₅ Cluster: Structural Analysis by Single Crystal X-ray Crystallography and Electron Nuclear Double Resonance. ACS Nano, 2014, 8, 3904-3912.	14.6	145
32	Atomistic Prediction of Sorption Free Energies of Cationic Aromatic Amines on Montmorillonite: A Linear Interaction Energy Method. Environmental Science and Technology Letters, 2014, 1, 284-289.	8.7	24
33	Thermodynamics of the Quasi-Epitaxial Flavin Assembly around Various-Chirality Carbon Nanotubes. Journal of the American Chemical Society, 2014, 136, 7452-7463.	13.7	23
34	Silicon Acceleration of a Tandem Alkene Isomerization/Electrocyclic Ring-opening of 2-Methyleneoxetanes to Î±,Î²-Unsaturated Methylketones. Journal of Organic Chemistry, 2013, 78, 11213-11220.	3.2	9
35	Interplay of Charge State, Lability, and Magnetism in the Molecule-like Au₂₅(SR)₁₈ Cluster. Journal of the American Chemical Society, 2013, 135, 15585-15594.	13.7	203
36	Recognition and Reactivity in the Binding between Raf Kinase Inhibitor Protein and Its Small-Molecule Inhibitor Locostatin. Journal of Physical Chemistry B, 2012, 116, 10176-10181.	2.6	12

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37	A QM/MM approach for the study of monolayer-protected gold clusters. Journal of Materials Science, 2012, 47, 7686-7692.	3.7	12
38	QM/MM Prediction of the Stark Shift in the Active Site of a Protein. Journal of Chemical Theory and Computation, 2012, 8, 2817-2823.	5.3	17
39	Stability of N-Glycosidic Bond of (5â€²S)-8,5â€²-Cyclo-2â€²-deoxyguanosine. Chemical Research in Toxicology, 2012, 25, 2451-2461.	3.3	21
40	Handedness Enantioselection of Carbon Nanotubes Using Helical Assemblies of Flavin Mononucleotide. Journal of the American Chemical Society, 2012, 134, 13196-13199.	13.7	40
41	Effect of the Charge State (z = â^'1, 0, +1) on the Nuclear Magnetic Resonance of Monodisperse Au₂₅[S(CH₂)₂Ph]₁₈^z Clusters. Analytical Chemistry, 2011, 83, 6355-6362.	6.5	124
42	Computational and experimental investigations of mono-septanoside binding by Concanavalin A: correlation of ligand stereochemistry to enthalpies of binding. Organic and Biomolecular Chemistry, 2011, 9, 154-164.	2.8	18
43	An extrapolation method for computing protein solvation energies based on density fragmentation of a graphical surface tessellation. Journal of Molecular Graphics and Modelling, 2011, 30, 38-45.	2.4	1
44	Shortâ€Circuiting Azobenzene Photoisomerization with Electronâ€Donating Substituents and Reactivating the Photochemistry with Chemical Modification. European Journal of Organic Chemistry, 2011, 2011, 2916-2919.	2.4	10
45	Locostatin Disrupts Association of Raf Kinase Inhibitor Protein With Binding Proteins by Modifying a Conserved Histidine Residue in the Ligand-Binding Pocket. Forum on Immunopathological Diseases and Therapeutics, 2011, 2, 47-58.	0.1	21
46	Proof for the Concerted Inversion Mechanism in the transâ†'cis Isomerization of Azobenzene Using Hydrogen Bonding To Induce Isomer Locking. Journal of Organic Chemistry, 2010, 75, 4817-4827.	3.2	79
47	QM/MM Approaches in Medicinal Chemistry Research. Current Topics in Medicinal Chemistry, 2010, 10, 46-54.	2.1	83
48	Unexpected Cleavage of 2-Azido-2-(hydroxymethyl)oxetanes: Conformation Determines Reaction Pathway?. Journal of Organic Chemistry, 2010, 75, 7565-7572.	3.2	13
49	Site-Preferential Dissociation of Peptides with Active Chemical Modification for Improving Fragment Ion Detection. Analytical Chemistry, 2010, 82, 23-27.	6.5	16
50	Molecular Modeling Characterization of a Conformationally Constrained Monolayer-Protected Gold Cluster. Journal of Physical Chemistry C, 2010, 114, 16043-16050.	3.1	11
51	The MoD-QM/MM methodology for structural refinement of photosystem II and other biological macromolecules. Photosynthesis Research, 2009, 102, 455-470.	2.9	41
52	Computational insights into the O2-evolving complex of photosystem II. Photosynthesis Research, 2008, 97, 91-114.	2.9	62
53	Optimization of cutting schemes for the evaluation of molecular electrostatic potentials in proteins via Moving-Domain QM/MM. Journal of Molecular Modeling, 2008, 14, 1-9.	1.8	15
54	QM/MM investigation of structure and spectroscopic properties of a vanadium-containing peroxidase. Journal of Inorganic Biochemistry, 2008, 102, 1684-1690.	3.5	32

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55	Synthesis and structureâ€“activity relationships of metalâ€“ligand complexes that potently inhibit cell migration. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 498-504.	2.2	45
56	Computational studies of the O2-evolving complex of photosystem II and biomimetic oxomanganese complexes. Coordination Chemistry Reviews, 2008, 252, 395-415.	18.8	146
57	A Model of the Oxygen-Evolving Center of Photosystem II Predicted by Structural Refinement Based on EXAFS Simulations. Journal of the American Chemical Society, 2008, 130, 6728-6730.	13.7	110
58	Quantum Mechanics/Molecular Mechanics Study of the Catalytic Cycle of Water Splitting in Photosystem II. Journal of the American Chemical Society, 2008, 130, 3428-3442.	13.7	345
59	QM/MM computational studies of substrate water binding to the oxygen-evolving centre of photosystem II. Philosophical Transactions of the Royal Society B: Biological Sciences, 2008, 363, 1149-1156.	4.0	70
60	Ligation Of The C-Terminus Of The D1 Polypeptide Of Photosystem Ii To The Oxygen Evolving Complex: A Dft-Qm/Mm Study. , 2008, , 363-368.		2
61	Quantum mechanics/molecular mechanics structural models of the oxygen-evolving complex of photosystem II. Current Opinion in Structural Biology, 2007, 17, 173-180.	5.7	91
62	A Self-Consistent Space-Domain Decomposition Method for QM/MM Computations of Protein Electrostatic Potentials. Journal of Chemical Theory and Computation, 2006, 2, 175-186.	5.3	47
63	Computational Studies of the Primary Phototransduction Event in Visual Rhodopsin. Accounts of Chemical Research, 2006, 39, 184-193.	15.6	75
64	QM/MM Models of the O2-Evolving Complex of Photosystem II. Journal of Chemical Theory and Computation, 2006, 2, 1119-1134.	5.3	136
65	Characterization of synthetic oxomanganese complexes and the inorganic core of the O2-evolving complex in photosystem II: Evaluation of the DFT/B3LYP level of theory. Journal of Inorganic Biochemistry, 2006, 100, 786-800.	3.5	99
66	SURFACE EFFECTS ON THE STATISTICS OF THE LOCAL DENSITY OF STATES IN METALLIC NANOPARTICLES: MANIFESTATION ON THE NMR SPECTRA. Modern Physics Letters B, 2005, 19, 1285-1294.	1.9	2
67	The mechanism of photosynthetic water splitting. Photochemical and Photobiological Sciences, 2005, 4, 940.	2.9	111
68	QM/MM Study of the NMR Spectroscopy of the Retinyl Chromophore in Visual Rhodopsin. Journal of Chemical Theory and Computation, 2005, 1, 674-685.	5.3	45
69	QM/MM Study of Energy Storage and Molecular Rearrangements Due to the Primary Event in Vision. Biophysical Journal, 2004, 87, 2931-2941.	0.5	98