Ricard Gelabert

List of Publications by Year
in descending order

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56	1,600	279798	302126
papers	citations	23 h-index	39 g-index

56	56	56	1495
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Semiclassical description of quantum coherence effects and their quenching: A forwardâ€“backward initial value representation study. Journal of Chemical Physics, 2001, 114, 2562-2571.	3.0	120
2	Electronic-structure and quantum dynamical study of the photochromism of the aromatic Schiff base salicylideneaniline. Journal of Chemical Physics, 2008, 129, 214308.	3.0	92
3	Rationally designed azobenzene photoswitches for efficient two-photon neuronal excitation. Nature Communications, 2019, 10, 907.	12.8	86
4	Potential Energy Landscape of the Photoinduced Multiple Proton-Transfer Process in the Green Fluorescent Protein:Â Classical Molecular Dynamics and Multiconfigurational Electronic Structure Calculations. Journal of the American Chemical Society, 2006, 128, 3564-3574.	13.7	80
5	Synthesis and Properties of Compressed Dihydride Complexes of Iridium:Â Theoretical and Spectroscopic Investigations. Journal of the American Chemical Society, 2004, 126, 8813-8822.	13.7	79
6	Semiclassical description of diffraction and its quenching by the forwardâ€“backward version of the initial value representation. Journal of Chemical Physics, 2001, 114, 2572-2579.	3.0	69
7	Elongated Dihydrogen Complexes:Â A Combined Electronic DFT + Nuclear Dynamics Study of the [Ru(HÂ·Â·Â·H)(C5H5)(H2PCH2PH2)]+Complex. Journal of the American Chemical Society, 1997, 119, 9840-9847.	13.7	64
8	Operation of the Proton Wire in Green Fluorescent Protein. A Quantum Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 5500-5511.	2.6	63
9	Theoretical Study on the Excited-State Intramolecular Proton Transfer in the Aromatic Schiff Base Salicylidene Methylamine:Â an Electronic Structure and Quantum Dynamical Approach. Journal of Physical Chemistry A, 2006, 110, 4649-4656.	2.5	57
10	Is an Extremely Low-Field Proton Signal in the NMR Spectrum Conclusive Evidence for a Low-Barrier Hydrogen Bond?. Journal of Physical Chemistry A, 1997, 101, 8727-8733.	2.5	55
11	Temperature Dependence of Proton NMR Chemical Shift As a Criterion To Identify Low-Barrier Hydrogen Bonds. Journal of the American Chemical Society, 1998, 120, 10203-10209.	13.7	53
12	Photo-deactivation pathways of a double H-bonded photochromic Schiff base investigated by combined theoretical calculations and experimental time-resolved studies. Physical Chemistry Chemical Physics, 2011, 13, 14960.	2.8	51
13	Are There Really Low-Barrier Hydrogen Bonds in Proteins? The Case of Photoactive Yellow Protein. Journal of the American Chemical Society, 2014, 136, 3542-3552.	13.7	51
14	Structure and Dynamics of LRhâ€œH4â€•(L = Cp, Tp) Systems. A Theoretical Study. Organometallics, 1997, 16, 3805-3814.	2.3	48
15	A Log-Derivative Formulation of the Prefactor for the Semiclassical Herman-Kluk Propagatorâ€. Journal of Physical Chemistry A, 2000, 104, 10321-10327.	2.5	47
16	Effect of the Spinning Motion of the Dihydrogen Ligand on the Properties of an Elongated Dihydrogen Complex. A Theoretical Study of the trans-[Os(HÂ·Â·Â·H)Cl(H2PCH2CH2PH2)2]+ Complex. Journal of the American Chemical Society, 1998, 120, 8168-8176.	13.7	45
17	A Potential Energy Function for Heterogeneous Proton-Wires. Ground and Photoactive States of the Proton-Wire in the Green Fluorescent Protein. Journal of Chemical Theory and Computation, 2008, 4, 1138-1150.	5.3	40
18	Quantum Dynamics Study of the Excited-State Double-Proton Transfer in 2,2â€²-Bipyridyl-3,3â€²-diol. ChemPhysChem, 2004, 5, 1372-1378.	2.1	37

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19	Determination of the Temperature Dependence of the Hâ^'D Spinâ^'Spin Coupling Constant and the Isotope Effect on the Proton Chemical Shift for the Compressed Dihydride Complex [Cp*Ir(Pâ^'P)H2]2+. Journal of the American Chemical Society, 2005, 127, 5632-5640.	13.7	37
20	A theoretical study of the photochemistry of indigo in its neutral and dianionic (leucoindigo) forms. Physical Chemistry Chemical Physics, 2013, 15, 20236.	2.8	37
21	Photoinduced proton transfer from the green fluorescent protein chromophore to a water molecule: analysis of the transfer coordinate. Chemical Physics Letters, 2004, 396, 202-207.	2.6	34
22	Charge-Transfer Ï€Ï€* Excited State in the 7-Azaindole Dimer. A Hybrid Configuration Interactions Singles/Time-Dependent Density Functional Theory Description. Journal of Physical Chemistry A, 2006, 110, 1145-1151.	2.5	30
23	Structure and Dynamics of [Nb(Î·5-C5H4SiMe3)2(Î·2-H2BR2)] (R2 = O2C6H4, C8H14, H2) Complexes. A Combined Experimental and Theoretical Study. Organometallics, 2000, 19, 3654-3663.	2.3	26
24	How Does the Environment Affect the Absorption Spectrum of the Fluorescent Protein mKeima?. Journal of Chemical Theory and Computation, 2013, 9, 1731-1742.	5.3	24
25	Electronic and quantum dynamical insight into the ultrafast proton transfer of 1-hydroxy-2-acetonaphthone. Journal of Chemical Physics, 2007, 127, 084318.	3.0	22
26	Elongated Dihydrogen Versus Compressed Dihydride Complexes: The Temperature Dependence of the H-D Spin-Spin Coupling Constant as a Criterion To Distinguish between Them. Chemistry - A European Journal, 2005, 11, 6315-6325.	3.3	20
27	Bipyridyl Derivatives as Photomemory Devices: A Comparative Electronicâ€Structure Study. Chemistry - A European Journal, 2010, 16, 6693-6703.	3.3	20
28	Nuclear Dynamics Discrete Variable Representation Study of the Equilibrium Isotope Effect on H2Binding in M(Î·2-H2)LnComplexes:Â An Effective Theoretical Way To Account for Anharmonicity. Journal of Physical Chemistry A, 2000, 104, 7898-7905.	2.5	19
29	A DVR analysis of some vibrational modes in the elongated dihydrogen complex [Ru(Î·2-H2)(C5H5)(H2PCH2PH2)]+. Chemical Physics, 1999, 241, 155-166.	1.9	17
30	Exploring the Effects of Intramolecular Vibrational Energy Redistribution on the Operation of the Proton Wire in Green Fluorescent Protein. Journal of Physical Chemistry B, 2008, 112, 13443-13452.	2.6	16
31	Peek at the Potential Energy Surfaces of the LSSmKate1 and LSSmKate2 Proteins. Journal of Physical Chemistry B, 2012, 116, 14302-14310.	2.6	16
32	Unveiling How an Archetypal Fluorescent Protein Operates: Theoretical Perspective on the Ultrafast Excited State Dynamics of GFP Variant S65T/H148D. Journal of Physical Chemistry B, 2015, 119, 2274-2291.	2.6	16
33	A Comparative Study on the Photochemistry of Two Bipyridyl Derivatives: [2,2â€²-Bipyridyl]-3,3â€²-diamine and [2,2â€²-Bipyridyl]-3,3â€²-diol. ChemPhysChem, 2007, 8, 1199-1206.	2.1	15
34	Transient low-barrier hydrogen bond in the photoactive state of green fluorescent protein. Physical Chemistry Chemical Physics, 2015, 17, 30876-30888.	2.8	14
35	Study of the Photochemical Properties and Conical Intersections of [2,2â€²â€Bipyridyl]â€3â€amineâ€3â€²â€ol. ChemPhysChem, 2008, 9, 2068-2076.	2.1	10
36	A time-dependent DFT/molecular dynamics study of the proton-wire responsible for the red fluorescence in the LSSmKate2 protein. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	10

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37	The Anomalous Isotope Effect for the Addition of Protium and Muonium to Pyrazine. A Theoretical Study. The Journal of Physical Chemistry, 1994, 98, 7858-7861.	2.9	9
38	Chromophore interactions leading to different absorption spectra in mNeptune1 and mCardinal red fluorescent proteins. Physical Chemistry Chemical Physics, 2016, 18, 16964-16976.	2.8	9
39	A variational transition state theory description of periselectivity effects on cycloadditions of ketenes with cyclopentadiene. Theoretical Chemistry Accounts, 2011, 128, 569-577.	1.4	7
40	Applicability of the WKB method in asymmetric double wells with degenerate and nondegenerate minima. Journal of Computational Chemistry, 1994, 15, 125-131.	3.3	6
41	The Quest for Photoswitches Activated by Nearâ€Infrared Light: A Theoretical Study of the Photochemistry of BF₂â€Coordinated Azo Derivatives. ChemPhysChem, 2016, 17, 2824-2838.	2.1	6
42	Semiclassical initial value representation description of molecular structure problems: An elongated dihydrogen ruthenium complex. Journal of Chemical Physics, 2002, 117, 7094-7101.	3.0	5
43	Modulating the Photochemistry of Bipyridylic Compounds by Symmetric Substitutions. ChemPhysChem, 2010, 11, 3696-3703.	2.1	5
44	New insights into the structureâ€“spectrum relationship in S65T/H148D and E222Q/H148D green fluorescent protein mutants: a theoretical assessment. Organic and Biomolecular Chemistry, 2014, 12, 9845-9852.	2.8	5
45	Deciphering the grounds of the suitability of acylhydrazones as efficient photoswitches. Physical Chemistry Chemical Physics, 2019, 21, 16075-16082.	2.8	5
46	Ultrafast action chemistry in slow motion: atomistic description of the excitation and fluorescence processes in an archetypal fluorescent protein. Physical Chemistry Chemical Physics, 2018, 20, 11067-11080.	2.8	4
47	A high-throughput computational approach to UV-Vis spectra in protein mutants. Physical Chemistry Chemical Physics, 2019, 21, 20678-20692.	2.8	4
48	On the unexpected isotope effect on the exchange coupling constant in partially deuterated transitionâ€metal trihydride complexes. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1998, 102, 354-358.	0.9	3
49	A Theoretical Assessment of Factors Causing Different Molecular Volumes in Isotopologues. Journal of Physical Chemistry A, 2009, 113, 14161-14169.	2.5	3
50	Theoretical Computerâ€Aided Mutagenic Study on the Triple Green Fluorescent Protein Mutant S65T/H148D/Y145F. ChemPhysChem, 2015, 16, 2134-2139.	2.1	3
51	Fast hydrogen elimination from the [Ru(PH3)3(CO)(H)2] complex in the first singlet excited states. A quantum dynamics study. Chemical Physics, 2003, 286, 149-163.	1.9	2
52	Molecular modelling of the pH influence in the geometry and the absorbance spectrum of near-infrared TagRFP675 fluorescent protein. Physical Chemistry Chemical Physics, 2015, 17, 29363-29373.	2.8	2
53	Tunnelling paths for proton transfer reactions in solution. A discussion over a simplified model. Computational and Theoretical Chemistry, 1996, 371, 161-169.	1.5	1
54	Isotope effects on the reaction of proton transfer to benzene anions in ethanol. Canadian Journal of Chemistry, 1997, 75, 1229-1233.	1.1	1

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55	A method to compute probability current in generic coordinates. Journal of Chemical Physics, 2011, 134, 074115.	3.0	0
56	A time-dependent DFT/molecular dynamics study of the proton-wire responsible for the red fluorescence in the LSSmKate2 protein. Highlights in Theoretical Chemistry, 2014, , 133-141.	0.0	0