JosÃ© M Lluch

List of Publications by Year
in descending order

282 papers	6,274 citations	71061 41 h-index	133188 59 g-index
289 all docs	289 docs citations	289 times ranked	4969 citing authors

#	Article	IF	Citations
1	Elongated dihydrogen complexes: what remains of the Hâ€“H Bond?. Chemical Society Reviews, 2004, 33, 175-182.	18.7	178
2	Theoretical Study of the Low-Barrier Hydrogen Bond in the Hydrogen Maleate Anion in the Gas Phase. Comparison with Normal Hydrogen Bonds. Journal of the American Chemical Society, 1997, 119, 1081-1086.	6.6	151
3	The use of quantum mechanics calculations for the study of corrosion inhibitors. Corrosion Science, 1984, 24, 929-933.	3.0	127
4	DNA Mutations Induced by Proton and Charge Transfer in the Low-Lying Excited Singlet Electronic States of the DNA Base Pairs:Â A Theoretical Insight. Journal of Physical Chemistry A, 1999, 103, 6251-6256.	1.1	104
5	Tunneling in Green Tea:Â Understanding the Antioxidant Activity of Catechol-Containing Compounds. A Variational Transition-State Theory Study. Journal of the American Chemical Society, 2007, 129, 5846-5854.	6.6	96
6	Electronic-structure and quantum dynamical study of the photochromism of the aromatic Schiff base salicylideneaniline. Journal of Chemical Physics, 2008, 129, 214308.	1.2	92
7	Theoretical study of molecular dynamics in model base pairs. Chemical Physics Letters, 1996, 256, 370-376.	1.2	90
8	Retaining Glycosyltransferase Mechanism Studied by QM/MM Methods: Lipopolysaccharyl-Î±-1,4-galactosyltransferase C Transfers Î±-Galactose via an Oxocarbenium Ion-like Transition State. Journal of the American Chemical Society, 2012, 134, 4743-4752.	6.6	89
9	H-Atom Transfer and Rotational Processes in the Ground and First Singlet Excited Electronic States of 2-(2â€˜-Hydroxyphenyl)oxazole Derivatives:Â Experimental and Theoretical Studiesâ€. The Journal of Physical Chemistry, 1996, 100, 19789-19794.	2.9	86
10	Rationally designed azobenzene photoswitches for efficient two-photon neuronal excitation. Nature Communications, 2019, 10, 907.	5.8	86
11	Bidimensional tunneling dynamics of malonaldehyde and hydrogenoxalate anion. A comparative study. Journal of Chemical Physics, 1990, 93, 5685-5692.	1.2	85
12	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.	6.6	80
13	Synthesis and Properties of Compressed Dihydride Complexes of Iridium:Â Theoretical and Spectroscopic Investigations. Journal of the American Chemical Society, 2004, 126, 8813-8822.	6.6	79
14	Ab Initio Based Exploration of the Potential Energy Surface for the Double Proton Transfer in the First Excited Singlet Electronic State of the 7-Azaindole Dimer. Journal of Physical Chemistry A, 2001, 105, 3887-3893.	1.1	70
15	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.	6.6	64
16	Operation of the Proton Wire in Green Fluorescent Protein. A Quantum Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 5500-5511.	1.2	63
17	Theoretical Study of the Hydrogen Exchange Coupling in the Metallocene Trihydride Complexes [(C5H5)2MH3]n+(M = Mo, W,n= 1; M = Nb, Ta,n= 0). Journal of the American Chemical Society, 1996, 118, 4617-4621.	6.6	60
18	Bidimensional tunneling splitting in the Aƒâ€‰1B2 and Xƒâ€‰1A1 states of tropolone. Journal of Chemical Physics, 1995, 103, 353-359.	1.2	58

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19	Synthesis and Spectroscopic Properties of Dihydrogen Isocyanide Niobocene [Nb(Î·5-C5H4SiMe3)2(Î·2-H2)(CNR)]+Complexes. Experimental and Theoretical Study of the Blocked Rotation of a Coordinated Dihydrogen. Journal of the American Chemical Society, 1997, 119, 6107-6114.	6.6	57
20	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.	1.1	57
21	Photoinduced Proton Transfer and Rotational Motion of 1-Hydroxy-2-acetonaphthone in the S1 State:â€‰ A Theoretical Insight into Its Photophysics. Journal of Physical Chemistry A, 2000, 104, 8424-8431.	1.1	56
22	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.	1.1	55
23	Evolutionary alteration of ALOX15 specificity optimizes the biosynthesis of antiinflammatory and proresolving lipoxins. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E4266-75.	3.3	54
24	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.	6.6	53
25	Determination of enzymatic reaction pathways using QM/MM methods. International Journal of Quantum Chemistry, 2003, 93, 229-244.	1.0	52
26	A Theoretical Analysis of Rate Constants and Kinetic Isotope Effects Corresponding to Different Reactant Valleys in Lactate Dehydrogenase. Journal of the American Chemical Society, 2006, 128, 16851-16863.	6.6	52
27	Asymmetry of the Hydrogen Bond of Hydrogen Phthalate Anion in Solution. A QM/MM Study. Journal of the American Chemical Society, 1999, 121, 9198-9207.	6.6	51
28	A theoretical study of the ground and first excited singlet state proton transfer reaction in isolated 7-azaindoleâ€“water complexes. Chemical Physics, 2003, 290, 319-336.	0.9	51
29	Enzyme Dynamics and Tunneling Enhanced by Compression in the Hydrogen Abstraction Catalyzed by Soybean Lipoxygenase-1. Journal of Physical Chemistry B, 2006, 110, 24708-24719.	1.2	51
30	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.	1.3	51
31	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.	6.6	51
32	Understanding the activation energy trends for the C2H4+OHâ†'C2H4OH reaction by using canonical variational transition state theory. Journal of Chemical Physics, 1997, 107, 7266-7274.	1.2	50
33	Variational Transition-State Theory with Optimized Orientation of the Dividing Surface and Semiclassical Tunneling Calculations for Deuterium and Muonium Kinetic Isotope Effects in the Free Radical Association Reaction H + C2H4 â†' C2H5. Journal of Physical Chemistry A, 1999, 103, 5061-5074.	1.1	50
34	On pKaMatching as a Requirement To Form a Low-Barrier Hydrogen Bond. A Theoretical Study in Gas Phase. Journal of Physical Chemistry A, 1997, 101, 3880-3886.	1.1	48
35	Structure and Dynamics of LRhâ€œH4â€•(L = Cp, Tp) Systems. A Theoretical Study. Organometallics, 1997, 16, 3805-3814.	1.1	48
36	Variational Transition State Theory and Tunneling Calculations with Reorientation of the Generalized Transition States for Methyl Cation Transfer. Journal of Physical Chemistry A, 1998, 102, 3420-3428.	1.1	48

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37	Quantum Mechanical Hydrogen Exchange Coupling in [(C5H5)Ir(L)H3]+ Complexes (L = PH3, CO). A Combined ab Initio/Tunneling Dynamics Study. Journal of the American Chemical Society, 1995, 117, 1069-1075.	6.6	46
38	Theoretical Modeling of Hydroxyl-Radical-Induced Lipid Peroxidation Reactions. Journal of Physical Chemistry B, 2007, 111, 5684-5693.	1.2	46
39	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.	6.6	45
40	The reactions CHnD4â^'n+OHâ†'P and CH4+ODâ†'CH3+HOD as a test of current direct dynamics computational methods to determine variational transition-state rate constants. I.. Journal of Chemical Physics, 2001, 114, 2154-2165.	1.2	44
41	Substrate-Assisted and Nucleophilically Assisted Catalysis in Bovine Î±1,3-Galactosyltransferase. Mechanistic Implications for Retaining Glycosyltransferases. Journal of the American Chemical Society, 2013, 135, 7053-7063.	6.6	42
42	Synthetic Photoswitchable Neurotransmitters Based on Bridged Azobenzenes. Organic Letters, 2019, 21, 3780-3784.	2.4	42
43	Variational Transition-State Theory Rate Constant Calculations with Multidimensional Tunneling Corrections of the Reaction of Acetone with OH. Journal of Physical Chemistry A, 2002, 106, 11760-11770.	1.1	40
44	Variational Transition State Theory as a Tool To Determine Kinetic Selectivity in Reactions Involving a Valley-Ridge Inflection Point. Journal of the American Chemical Society, 2004, 126, 13089-13094.	6.6	40
45	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.	2.3	40
46	Theoretical Study of the Mechanism of the Hydride Transfer between Ferredoxinâ€"NADP⁺ Reductase and NADP⁺: The Role of Tyr303. Journal of the American Chemical Society, 2012, 134, 20544-20553.	6.6	40
47	Theoretical study of solvation effects on chemical reactions. A combined quantum chemical/Monte Carlo study of the Meyer-Schuster reaction mechanism in water. Journal of the American Chemical Society, 1989, 111, 829-835.	6.6	39
48	Unraveling How Enzymes Can Use Bulky Residues To Drive Site-Selective Câ€"H Activation: The Case of Mammalian Lipoxygenases Catalyzing Arachidonic Acid Oxidation. ACS Catalysis, 2014, 4, 4351-4363.	5.5	39
49	A computational and experimental study of O-glycosylation. Catalysis by human UDP-GalNAc polypeptide:GalNAc transferase-T2. Organic and Biomolecular Chemistry, 2014, 12, 2645-2655.	1.5	39
50	A QM/MM Study of the Racemization of Vinylglycolate Catalyzed by Mandelate Racemase Enzyme. Journal of the American Chemical Society, 2001, 123, 709-721.	6.6	38
51	On the intramolecular proton transfer of 3-hydroxyflavone in the first singlet excited state: A theoretical study. Chemical Physics, 2006, 325, 243-250.	0.9	38
52	Quantum Dynamics Study of the Excited-State Double-Proton Transfer in 2,2â€²-Bipyridyl-3,3â€²-diol. ChemPhysChem, 2004, 5, 1372-1378.	1.0	37
53	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.	6.6	37
54	A theoretical study of the photochemistry of indigo in its neutral and dianionic (leucoindigo) forms. Physical Chemistry Chemical Physics, 2013, 15, 20236.	1.3	37

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55	Tunneling dynamics in isotopically substituted malonaldehyde. Comparison between symmetric and asymmetric species. Journal of the American Chemical Society, 1992, 114, 2072-2076.	6.6	35
56	Testing electronic structure methods for describing intermolecular H Â· Â· Â· H interactions in supramolecular chemistry. Journal of Computational Chemistry, 2004, 25, 99-105.	1.5	35
57	A Native Ternary Complex Trapped in a Crystal Reveals the Catalytic Mechanism of a Retaining Glycosyltransferase. Angewandte Chemie - International Edition, 2015, 54, 9898-9902.	7.2	35
58	Mechanism of the Gas-Phase HO + H2O â†' H2O + OH Reaction and Several Associated Isotope Exchange Reactions:â€‰ A Canonical Variational Transition State Theory Plus Multidimensional Tunneling Calculation. Journal of Physical Chemistry A, 1999, 103, 1044-1053.	1.1	34
59	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.	1.2	34
60	The regioselectivity of 4-nitroanisole photosubstitution with primary amines. A mechanistic and theoretical study. Journal of Organic Chemistry, 1990, 55, 3303-3310.	1.7	33
61	On the Ionization State of the Substrate in the Active Site of Glutamate Racemase. A QM/MM Study about the Importance of Being Zwitterionicâ€. Journal of Physical Chemistry A, 2006, 110, 717-725.	1.1	33
62	Searching for Saddle Points by Using the Nudged Elastic Band Method:â€‰ An Implementation for Gas-Phase Systems. Journal of Chemical Theory and Computation, 2006, 2, 895-904.	2.3	33
63	Ligandâ€‰induced formation of transient dimers of mammalian 12/15â€‰lipoxygenase: A key to allosteric behavior of this class of enzymes?. Proteins: Structure, Function and Bioinformatics, 2012, 80, 703-712.	1.5	33
64	Understanding the Mechanism of the Hydrogen Abstraction from Arachidonic Acid Catalyzed by the Human Enzyme 15-Lipoxygenase-2. A Quantum Mechanics/Molecular Mechanics Free Energy Simulation. Journal of Chemical Theory and Computation, 2016, 12, 2079-2090.	2.3	33
65	Ab initio calculations of the quantum mechanical hydrogen exchange coupling in the [(C5H5)Ir(PH3)H3]+ complex. Journal of the American Chemical Society, 1993, 115, 5861-5862.	6.6	32
66	On the experimental evidences for 7-azaindole base-pair model ultrafast phototautomerization. Chemical Physics Letters, 2000, 324, 81-87.	1.2	31
67	A Monte Carlo simulation of Fe2+ aqueous solvation. Chemical Physics, 1987, 111, 241-247.	0.9	30
68	Entropic Effects on the Dynamical Bottleneck Location and Tunneling Contributions for C2H4 + H â†' C2H5:â€‰ Variable Scaling of External Correlation Energy for Association Reactions. Journal of the American Chemical Society, 1998, 120, 5559-5567.	6.6	30
69	Variational Transition-State Theory Rate Constant Calculations of the OH + CH3SH Reaction and Several Isotopic Variants. Journal of Physical Chemistry A, 2003, 107, 4490-4496.	1.1	30
70	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.	1.1	30
71	Insights into the Mechanism of Binding of Arachidonic Acid to Mammalian 15-Lipoxygenases. Journal of Physical Chemistry B, 2010, 114, 7037-7046.	1.2	30
72	Topologically Controlled Coulombic Interactions, a New Tool in the Developing of Novel Reactivity. Photochemical and Electrochemical Cleavage of Phenyl Alkyl Ethers. Journal of Organic Chemistry, 1995, 60, 3814-3825.	1.7	29

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73	The reactions CHnD4âˆ'n+OHâ†'P and CH4+ODâ†'CH3+HOD as a test of current direct dynamics multicoefficient methods to determine variational transition state rate constants. II. Journal of Chemical Physics, 2001, 115, 4515-4526.	1.2	29
74	A Fast Radical Chain Mechanism in the Polyfluoroalkoxylation of Aromatics through NO2 Group Displacement. Mechanistic and Theoretical Studies. Journal of Organic Chemistry, 2005, 70, 1718-1727.	1.7	29
75	Nitrophenyl ethers as possible photoaffinity labels. The nucleophilic aromatic photosubstitution revisited.. Tetrahedron Letters, 1984, 25, 4147-4150.	0.7	28
76	The nucleophilic aromatic photosubstitutions of 4,5-dinitroveratrole with amines. Tetrahedron, 1987, 43, 351-360.	1.0	28
77	A theoretical insight into the internal H-bond and related rotational motion and proton transfer processes of 1-hydroxy-2-acetonaphthone in the S0 state. Chemical Physics Letters, 2000, 328, 83-89.	1.2	28
78	Thermodynamics, Kinetics, and Dynamics of the Two Alternative Aniomesolytic Fragmentations of Câ'O Bonds:â€‰ An Electrochemical and Theoretical Study. Journal of the American Chemical Society, 2002, 124, 4708-4715.	6.6	28
79	On the theoretical reports on 7-azaindole base-pair phototautomerization. Chemical Physics Letters, 2000, 324, 75-80.	1.2	27
80	Electronic structure study of the initiation routes of the dimethyl sulfide oxidation by OH. Journal of Computational Chemistry, 2005, 26, 569-583.	1.5	27
81	Mechanism of the Hydride Transfer between Anabaena Tyr303Ser FNR_{rd}/FNR_{ox} and NADP⁺/H. A Combined Pre-Steady-State Kinetic/Ensemble-Averaged Transition-State Theory with Multidimensional Tunneling Study. Journal of Physical Chemistry B, 2010, 114, 3368-3379.	1.2	27
82	A semiclassical simulation for tunneling dynamics of malonaldehyde and hydrogenoxalate anion. Chemical Physics, 1992, 159, 99-107.	0.9	26
83	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.	1.1	26
84	Geometry optimization and transition state search in enzymes: Different options in the microiterative method. International Journal of Quantum Chemistry, 2004, 98, 367-377.	1.0	26
85	The curvature of the Arrhenius plots predicted by conventional canonical transition-state theory in the absence of tunneling. Theoretical Chemistry Accounts, 2003, 110, 352-357.	0.5	25
86	A QM/MM study of the phosphoryl transfer to the Kemptide substrate catalyzed by protein kinase A. The effect of the phosphorylation state of the protein on the mechanism. Physical Chemistry Chemical Physics, 2011, 13, 530-539.	1.3	25
87	Intrinsic reaction coordinate calculations for reaction paths possessing branching points. Chemical Physics Letters, 1989, 160, 543-548.	1.2	24
88	Ab initio study of the ground and lowâ€‹ying states of FeH. Journal of Chemical Physics, 1990, 92, 2478-2480.	1.2	24
89	How Does the Environment Affect the Absorption Spectrum of the Fluorescent Protein mKeima?. Journal of Chemical Theory and Computation, 2013, 9, 1731-1742.	2.3	24
90	The effect of the correlation energy on the mechanism of the Dielsâ€"Alder reaction. Chemical Physics Letters, 1983, 102, 317-320.	1.2	23

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91	Solvent effect in the Walden inversion reactions. Chemical Physics Letters, 1984, 106, 232-236.	1.2	23
92	The role of many-body interactions in the stability of hydrated Cu2+ clusters. Chemical Physics, 1990, 141, 379-392.	0.9	23
93	Dihydrogen Formation in a Trihydride Metallocene and Its Elimination, Both Assisted by Lewis Acids: The[Cp2NbH3]+BH3 System. Angewandte Chemie International Edition in English, 1997, 36, 265-266.	4.4	23
94	Reaction-Path and Dual-Level Dynamics Calculations of the CH3F + OH Reaction. Journal of Physical Chemistry A, 1998, 102, 10715-10722.	1.1	23
95	Photo-oxidation of lipids by singlet oxygen: a theoretical study. Chemical Physics Letters, 2004, 398, 336-342.	1.2	23
96	Variational Transition-State Theory Study of the Dimethyl Sulfoxide (DMSO) and OH Reactionâ€. Journal of Physical Chemistry A, 2006, 110, 798-808.	1.1	23
97	How the Substrate d-Glutamate Drives the Catalytic Action of Bacillus subtilis Glutamate Racemase. Journal of the American Chemical Society, 2009, 131, 3509-3521.	6.6	23
98	Molecular Dynamics of Excited State Intramolecular Proton Transfer:â€‰ 2-(2â€˜-Hydroxyphenyl)-4-methyloxazole in Gas Phase, Solution, and Protein Environments. Journal of Physical Chemistry B, 2004, 108, 6616-6623.	1.2	22
99	A QM/MM Exploration of the Potential Energy Surface of Pyruvate to Lactate Transformation Catalyzed by LDH. Improving the Accuracy of Semiempirical Descriptions. Journal of Chemical Theory and Computation, 2005, 1, 750-761.	2.3	22
100	Electronic and quantum dynamical insight into the ultrafast proton transfer of 1-hydroxy-2-acetonaphthone. Journal of Chemical Physics, 2007, 127, 084318.	1.2	22
101	Computational insight into the catalytic implication of head/tail-first orientation of arachidonic acid in human 5-lipoxygenase: consequences for the positional specificity of oxygenation. Physical Chemistry Chemical Physics, 2016, 18, 23017-23035.	1.3	22
102	Symmetric intramolecular proton transfers between oxygen atoms in anionic systems. An ab initio study. Journal of the American Chemical Society, 1990, 112, 3868-3874.	6.6	21
103	Theoretical study of the role of arginine 127 in the water-promoted mechanism of peptide cleavage by carboxypeptidase A. New Journal of Chemistry, 1998, 22, 319-326.	1.4	21
104	Variational Transition State Calculations of the CH2F2 + OH Hydrogen Abstraction Reaction. Journal of Physical Chemistry A, 2001, 105, 10553-10561.	1.1	21
105	A combined nuclear dynamics and electronic study of the coupling between the internal rotation of the methyl group and the intramolecular proton transfer in 5-methyltropolone. Journal of Chemical Physics, 2002, 117, 7525-7533.	1.2	21
106	Kinetic isotope effects in chemical and biochemical reactions: physical basis and theoretical methods of calculation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 584-603.	6.2	21
107	Explanation of Deuterium and Muonium Kinetic Isotope Effects for Hydrogen Atom Addition to an Olefin. Journal of the American Chemical Society, 1998, 120, 12141-12142.	6.6	20
108	Hydrogen Abstraction by Soybean Lipoxygenase-1. Density Functional Theory Study on Active Site Models in Terms of Gibbs Free Energies. Journal of Physical Chemistry B, 2004, 108, 13831-13838.	1.2	20

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109	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.	1.7	20
110	Bipyridyl Derivatives as Photomemory Devices: A Comparative Electronicâ€Structure Study. Chemistry - A European Journal, 2010, 16, 6693-6703.	1.7	20
111	Discovery of processive catalysis by an exo-hydrolase with a pocket-shaped active site. Nature Communications, 2019, 10, 2222.	5.8	20
112	Ground and lowâ€lying states of FeH+ as derived from ab initio selfâ€consistent field and configuration interaction calculations. Journal of Chemical Physics, 1989, 90, 6436-6442.	1.2	19
113	Use of intramolecular coulombic interactions to achieve impossible reactions. Photochemical cleavage of 4-nitrophenyl ethers. Journal of the American Chemical Society, 1991, 113, 8970-8972.	6.6	19
114	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.	1.1	19
115	SP20 Phosphorylation Reaction Catalyzed by Protein Kinase A: QM/MM Calculations Based on Recently Determined Crystallographic Structures. ACS Catalysis, 2015, 5, 4897-4912.	5.5	19
116	Inhibition of Mammalian 15-Lipoxygenase by Three Ebselen-like Drugs. A QM/MM and MM/PBSA Comparative Study. Journal of Physical Chemistry A, 2017, 121, 9752-9763.	1.1	19
117	Ab initio study of the NH3 + OH reaction. Chemical Physics, 1992, 165, 41-46.	0.9	18
118	On the water-promoted mechanism of peptide cleavage by carboxypeptidase A. A theoretical study. Canadian Journal of Chemistry, 1994, 72, 2077-2083.	0.6	18
119	On the photoisomerization of 5-hydroxytropolone: An abâ€‰initio and nuclear wave function study. Journal of Chemical Physics, 1997, 107, 6275-6282.	1.2	18
120	A QM/MM study of Kemptide phosphorylation catalyzed by protein kinase A. The role of Asp166 as a general acid/base catalyst. Physical Chemistry Chemical Physics, 2015, 17, 3497-3511.	1.3	18
121	How Can Linoleic Acid Be the Preferential Substrate of the Enzyme 15-Lipoxygenase-1? A QM/MM Approach. Journal of Physical Chemistry B, 2016, 120, 1950-1960.	1.2	18
122	Comparing Hydrolysis and Transglycosylation Reactions Catalyzed by Thermus thermophilus Î²-Glycosidase. A Combined MD and QM/MM Study. Frontiers in Chemistry, 2019, 7, 200.	1.8	18
123	A DVR analysis of some vibrational modes in the elongated dihydrogen complex [Ru(Î·2-H2)(C5H5)(H2PCH2PH2)]+. Chemical Physics, 1999, 241, 155-166.	0.9	17
124	Effect of a complex formation on the calculated low-pressure rate constant of a bimolecular gas-phase reaction governed by tunneling. Journal of Computational Chemistry, 1999, 20, 1685-1692.	1.5	17
125	Effective way of modeling chemical catalysis: Empirical valence bond picture of role of solvent and catalyst in alkylation reactions. Journal of Computational Chemistry, 2000, 21, 607-625.	1.5	17
126	Theoretical study of the photoinduced intramolecular proton transfer and rotational processes in 2-(2â€²hydroxyphenyl)-4-methyloxazole in gas phase and embedded in Î²-cyclodextrin. Journal of Photochemistry and Photobiology A: Chemistry, 2005, 173, 365-374.	2.0	17

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127	Essential role of glutamate 317 in galactosyl transfer by Î±3GalT: a computational study. Carbohydrate Research, 2012, 356, 204-208.	1.1	17
128	An Insight into the Regiospecificity of Linoleic Acid Peroxidation Catalyzed by Mammalian 15-Lipoxygenases. Journal of Physical Chemistry B, 2013, 117, 3747-3754.	1.2	17
129	Understanding the Molecular Mechanism of the Ala-versus-Gly Concept Controlling the Product Specificity in Reactions Catalyzed by Lipoxygenases: A Combined Molecular Dynamics and QM/MM Study of Coral 8R-Lipoxygenase. ACS Catalysis, 2017, 7, 4854-4866.	5.5	17
130	Theoretical study of the conformational preferences in the Cl4W:CH2 complex. Organometallics, 1989, 8, 1837-1841.	1.1	16
131	The search for stationary points on a quantum mechanical/molecular mechanical potential-energy surface. Theoretical Chemistry Accounts, 2002, 107, 147-153.	0.5	16
132	Canonical Variational Transition-State Theory Study of the CF3CH2CH3 + OH Reaction. Journal of Physical Chemistry B, 2008, 112, 328-335.	1.2	16
133	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.	1.2	16
134	Peek at the Potential Energy Surfaces of the LSSmKate1 and LSSmKate2 Proteins. Journal of Physical Chemistry B, 2012, 116, 14302-14310.	1.2	16
135	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.	1.2	16
136	Excited states and electronic spectra of monosubstituted benzenes. An AM1 study. Spectrochimica Acta Part A: Molecular Spectroscopy, 1988, 44, 1427-1434.	0.1	15
137	A Monte Carlo Simulation of the Electrochemical Reduction of Alkyl Halides in Water. On the Validity of Marcus' Relationship. Journal of the American Chemical Society, 1994, 116, 10117-10123.	6.6	15
138	Theoretical Study of the Effect of Lewis Acids on Dihydrogen Elimination from Niobocene Trihydrides. Chemistry - A European Journal, 1999, 5, 1166-1171.	1.7	15
139	The photoinduced intramolecular proton transfer in 2-(2â€²-hydroxyphenyl)-4-methyloxazole embedded in Î²-cyclodextrin. Chemical Physics Letters, 2002, 356, 423-430.	1.2	15
140	A PM3/d specific reaction parameterization for iron atom in the hydrogen abstraction catalyzed by soybean lipoxygenase-1. Journal of Computational Chemistry, 2007, 28, 997-1005.	1.5	15
141	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.	1.0	15
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