Ines Corral

List of Publications by Year
in descending order

111 papers	4,333 citations	185998 28 h-index	110170 64 g-index
116 all docs	116 docs citations	116 times ranked	3058 citing authors

#	Article	IF	Citations
1	Critical appraisal of the fewest switches algorithm for surface hopping. Journal of Chemical Physics, 2007, 126, 134114.	1.2	524
2	The on-the-fly surface-hopping program system Newton-X: Application to ab initio simulation of the nonadiabatic photodynamics of benchmark systems. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 228-240.	2.0	422
3	Newtonâ€<scp>X</scp>: a surfaceâ€hopping program for nonadiabatic molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 26-33.	6.2	370
4	Including quantum decoherence in surface hopping. Journal of Chemical Physics, 2010, 133, 134111.	1.2	309
5	Surface hopping dynamics using a locally diabatic formalism: Charge transfer in the ethylene dimer cation and excited state dynamics in the 2-pyridone dimer. Journal of Chemical Physics, 2012, 137, 22A514.	1.2	173
6	An overview of nonadiabatic dynamics simulations methods, with focus on the direct approach versus the fitting of potential energy surfaces. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	158
7	The origin of efficient triplet state population in sulfur-substituted nucleobases. Nature Communications, 2016, 7, 13077.	5.8	149
8	Photodynamics and Time-Resolved Fluorescence of Azobenzene in Solution: A Mixed Quantum-Classical Simulation. Journal of the American Chemical Society, 2011, 133, 5109-5123.	6.6	140
9	Competing ultrafast intersystem crossing and internal conversion: a time resolved picture for the deactivation of 6-thioguanine. Chemical Science, 2014, 5, 1336.	3.7	126
10	Surface hopping trajectory simulations with spin-orbit and dynamical couplings. Journal of Chemical Physics, 2012, 137, 22A501.	1.2	122
11	Molecular gradients for semiempirical CI wavefunctions with floating occupation molecular orbitals. Chemical Physics Letters, 2000, 325, 79-85.	1.2	116
12	An ab initio mechanism for efficient population of triplet states in cytotoxic sulfur substituted DNA bases: the case of 6-thioguanine. Chemical Communications, 2012, 48, 2134.	2.2	76
13	Electronic and Structural Elements That Regulate the Excited-State Dynamics in Purine Nucleobase Derivatives. Journal of the American Chemical Society, 2015, 137, 4368-4381.	6.6	72
14	Semiempirical Hamiltonian for Simulation of Azobenzene Photochemistry. Journal of Physical Chemistry A, 2012, 116, 98-110.	1.1	62
15	An Experimental and Theoretical Investigation of Gas-Phase Reactions of Ca2+ with Glycine. Chemistry - A European Journal, 2006, 12, 6787-6796.	1.7	57
16	Photophysics and Photochemistry of Canonical Nucleobasesâ€™ Thioanalogs: From Quantum Mechanical Studies to Time Resolved Experiments. Molecules, 2017, 22, 998.	1.7	57
17	Hybrid-Basis Close-Coupling Interface to Quantum Chemistry Packages for the Treatment of Ionization Problems. Journal of Chemical Theory and Computation, 2017, 13, 499-514.	2.3	54
18	Decoding the Molecular Basis for the Population Mechanism of the Triplet Phototoxic Precursors in UVA Lightâ€Activated Pyrimidine Anticancer Drugs. Chemistry - A European Journal, 2017, 23, 2619-2627.	1.7	49

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19	Gas-Phase Reactions between Urea and Ca2+:Â The Importance of Coulomb Explosions. Journal of Physical Chemistry A, 2004, 108, 10080-10088.	1.1	48
20	Simulation of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si109.gif" overflow="scroll"><mml:mrow><mml:mi>Ï€</mml:mi><mml:mo>â†'</mml:mo><mml:msup><mml:mrow><mml:mi>Ï€</mml:mi></mml: photodynamics of azobenzene: Decoherence and solvent effects. Computational and Theoretical Chemistry, 2014, 1040-1041, 126-135.	1.1	43
21	Interactions between Neutral Molecules and Ca2+:â€‰ An Assessment of Theoretical Procedures. Journal of Physical Chemistry A, 2003, 107, 10456-10461.	1.1	42
22	An Insight into the Mechanism of the Axial Ligand Exchange Reaction in Boron Subphthalocyanine Macrocycles. Journal of the American Chemical Society, 2014, 136, 14289-14298.	6.6	42
23	Agostic vs Ï€-Interactions in Complexes of Ethynylsilanes and Ethynylgermanes with Cu+in the Gas Phase. Journal of Physical Chemistry A, 2003, 107, 1370-1376.	1.1	37
24	Ultrafast irreversible phototautomerization of o-nitrobenzaldehyde. Chemical Communications, 2011, 47, 6383.	2.2	33
25	Dynamics of acetone photodissociation: a surface hopping study. Physical Chemistry Chemical Physics, 2013, 15, 20651.	1.3	32
26	Photodynamics of azobenzene in a hindering environment. Chemical Physics, 2008, 347, 492-502.	0.9	31
27	Versatile Bottomâ€up Approach to Stapled Ï€â€Conjugated Helical Scaffolds: Synthesis and Chiroptical Properties of Cyclic oâ€Phenylene Ethynylene Oligomers. Angewandte Chemie - International Edition, 2012, 51, 13036-13040.	7.2	31
28	Electronic States of o-Nitrobenzaldehyde: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 5046-5053.	1.1	30
29	Multiscale Models for Light-Driven Processes. Annual Review of Physical Chemistry, 2021, 72, 489-513.	4.8	29
30	Surface hopping investigation of benzophenone excited state dynamics. Physical Chemistry Chemical Physics, 2016, 18, 10499-10506.	1.3	28
31	Cu+ association to some Phâ€“X (X=OH, NH2, CHO, COOH, CF3) phenyl derivatives.. International Journal of Mass Spectrometry, 2006, 255-256, 20-27.	0.7	27
32	Binding energies of Cu+ to saturated and Î±,Î²-unsaturated alkanes, silanes and germanes. International Journal of Mass Spectrometry, 2003, 227, 401-412.	0.7	26
33	Interplay of radiative and nonradiative transitions in surface hopping with radiation-molecule interactions. Journal of Chemical Physics, 2014, 140, 044113.	1.2	26
34	Direct Access to Axially Substituted Subphthalocyanines from Trimethylsilyl-Protected Nucleophiles. Organic Letters, 2015, 17, 4722-4725.	2.4	26
35	Turn-on Fluorescent Biosensors for Imaging Hypoxia-like Conditions in Living Cells. Journal of the American Chemical Society, 2022, 144, 8185-8193.	6.6	26
36	Annulated Dinuclear Metal-Free and Zn(II) Phthalocyanines: Photophysical Studies and Quantum Mechanical Calculations. Journal of Physical Chemistry B, 2008, 112, 8466-8476.	1.2	25

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37	Photochemistry in the strong coupling regime: A trajectory surface hopping scheme. Journal of Computational Chemistry, 2020, 41, 2033-2044.	1.5	25
38	The oxidation state in low-valent beryllium and magnesium compounds. Chemical Science, 2022, 13, 6583-6591.	3.7	25
39	Gradients for configuration interaction energies with spinâ€orbit coupling in a semiempirical framework. Journal of Computational Chemistry, 2011, 32, 2690-2696.	1.5	24
40	Berylliumâ€Based Anion Sponges: Close Relatives of Proton Sponges. Chemistry - A European Journal, 2016, 22, 18322-18325.	1.7	24
41	Super Strong Beâ€“Be Bonds: Theoretical Insight into the Electronic Structure of Beâ€“Be Complexes with Radical Ligands. Journal of Physical Chemistry A, 2018, 122, 2258-2265.	1.1	23
42	Beyond the Classical Electronâ€Sharing and Dative Bond Picture: Case of the Spinâ€Polarized Bond. Angewandte Chemie - International Edition, 2021, 60, 1498-1502.	7.2	23
43	Exergonic and Spontaneous Production of Radicals through Beryllium Bonds. Angewandte Chemie - International Edition, 2016, 55, 8736-8739.	7.2	22
44	The Role of Electronic Triplet States and Highâ€Lying Singlet States in the Deactivation Mechanism of the Parent BODIPY: An ADC(2) and CASPT2 Study. ChemPhotoChem, 2019, 3, 727-738.	1.5	21
45	The importance of agostic-type interactions for the binding energies of Ni+to saturated and Î±,Î²-unsaturated alkanes, silanes and germanes. New Journal of Chemistry, 2003, 27, 1657-1664.	1.4	20
46	Time-Resolved Insight into the Photosensitized Generation of Singlet Oxygen in Endoperoxides. Journal of Chemical Theory and Computation, 2015, 11, 406-414.	2.3	20
47	Four Plus Four State Degeneracies in the Oâ^'O Photolysis of Aromatic Endoperoxides. Journal of Physical Chemistry Letters, 2010, 1, 1036-1040.	2.1	19
48	Some Pictures of Alcoholic Dancing: From Simple to Complex Hydrogen-Bonded Networks Based on Polyalcohols. Journal of Physical Chemistry C, 2013, 117, 4680-4690.	1.5	18
49	Potential Energy Surfaces of Core-Hole and Shake-Up States for Dissociative Ionization Studies. Journal of Chemical Theory and Computation, 2017, 13, 1723-1736.	2.3	18
50	Identifying the low-lying electronic states of anthracene-9,10-endoperoxide. Chemical Physics Letters, 2008, 452, 67-71.	1.2	17
51	Density functional theory rationalization of the substituent effects in trifluoromethyl-pyridinol derivatives. Tetrahedron, 2009, 65, 232-239.	1.0	17
52	A non-adiabatic quantum-classical dynamics study of the intramolecular excited state hydrogen transfer in ortho-nitrobenzaldehyde. Physical Chemistry Chemical Physics, 2011, 13, 14685.	1.3	17
53	A comparative analysis of the UV/Vis absorption spectra of nitrobenzaldehydes. Physical Chemistry Chemical Physics, 2011, 13, 4269.	1.3	17
54	Development of a New Dual Polarity and Viscosity Probe Based on the Foldamer Concept. Organic Letters, 2015, 17, 2844-2847.	2.4	17

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55	Why Are the Ca2+ and K+ Binding Energies of Formaldehyde and Ammonia Reversed with Respect to Their Proton Affinities?. Journal of Physical Chemistry A, 2005, 109, 6735-6742.	1.1	16
56	Theoretical investigation of anthraceneâ€9,10â€endoperoxide vertical singlet and triplet excitation spectra. Journal of Computational Chemistry, 2008, 29, 1982-1991.	1.5	15
57	On the existence and lifetimes of Cu2+ complexes with water, ammonia, and hydrogen cyanide. Journal of Chemical Physics, 2005, 123, 014315.	1.2	14
58	Four-state conical intersections: The nonradiative deactivation funnel connected to Oâ€“O homolysis in benzene endoperoxide. Chemical Physics Letters, 2010, 499, 21-25.	1.2	13
59	[MLn]2+ doubly charged systems: modeling, bonding, life times and unimolecular reactivity. Physical Chemistry Chemical Physics, 2011, 13, 14848.	1.3	13
60	Sub-laser-cycle control of coupled electronâ€“nuclear dynamics at a conical intersection. New Journal of Physics, 2015, 17, 113023.	1.2	13
61	Excited state dynamics of some nonsteroidal anti-inflammatory drugs: A surface-hopping investigation. Computational and Theoretical Chemistry, 2019, 1152, 20-27.	1.1	13
62	Surface Hopping Dynamics with the Frenkel Exciton Model in a Semiempirical Framework. Journal of Chemical Theory and Computation, 2021, 17, 7373-7383.	2.3	13
63	Quantum and semiclassical dynamics of the Franckâ€“Condon wave packet on the coupled potential surfaces of the conical intersection. Chemical Physics, 2000, 259, 193-200.	0.9	11
64	The importance of nonconventional structures in the binding of Ni+ to ethynylsilanes and ethynylgermanes. Theoretical Chemistry Accounts, 2004, 112, 298.	0.5	10
65	The electronic excited states of a model organic endoperoxide: A comparison of TD-DFT and ab initio methods. Chemical Physics Letters, 2007, 446, 262-267.	1.2	10
66	Electronic structure and lifetimes of GaX2+ (X = N, O, F) in the gas phase. Unraveling stability trends. Physical Chemistry Chemical Physics, 2011, 13, 18365.	1.3	10
67	Beryllium-based fluorenes as efficient anion sponges. Physical Chemistry Chemical Physics, 2017, 19, 23052-23059.	1.3	10
68	Nonadiabatic scattering of NO off Au₃ clusters: A simple and robust diabatic state manifold generation method for multiconfigurational wavefunctions. Journal of Computational Chemistry, 2019, 40, 794-810.	1.5	10
69	On the Origin of the Photostability of DNA and RNA Monomers: Excited State Relaxation Mechanism of the Pyrimidine Chromophore. Journal of Physical Chemistry Letters, 2020, 11, 5156-5161.	2.1	10
70	Theoretical investigation of a novel xylene-based light-driven unidirectional molecular motor. Journal of Chemical Physics, 2021, 154, 064111.	1.2	10
71	Infrared spectra of chargeâ€solvated versus saltâ€bridge conformations of glycineâ€, serineâ€, and cysteineâ€Ca²⁺ complexes. International Journal of Quantum Chemistry, 2012, 112, 2126-2134.	1.0	9
72	Exergonic and Spontaneous Production of Radicals through Beryllium Bonds. Angewandte Chemie, 2016, 128, 8878-8881.	1.6	9

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73	Tracking the origin of photostability in purine nucleobases: the photophysics of 2-oxopurine. Physical Chemistry Chemical Physics, 2019, 21, 13467-13473.	1.3	9
74	Li+ vs Cu+ Association to Toluene, Phenylsilane and Phenylgermane. Conventional vs Non-Conventional Ï€-Complexes. European Journal of Mass Spectrometry, 2004, 10, 921-929.	0.5	8
75	Hydrogen bonding in electronically excited states: a comparison between formic acid dimer and its mono-substituted thioderivatives. Physical Chemistry Chemical Physics, 2010, 12, 13037.	1.3	8
76	On the stability and lifetime of GaO2+ in the gas phase. Theoretical Chemistry Accounts, 2011, 129, 401-407.	0.5	8
77	Mesityl or Imide Acridinium Photocatalysts: Accessible Versus Inaccessible Chargeâ€Transfer States in Photoredox Catalysis. ChemPhotoChem, 2019, 3, 609-612.	1.5	8
78	Interplay between the Directing Group and Multifunctional Acetate Ligand in Pd-Catalyzed anti-Acetoxylation of Unsymmetrical Dialkyl-Substituted Alkynes. ACS Catalysis, 2022, 12, 6596-6605.	5.5	8
79	Unexpected Gas-Phase Ion Chemistry Results Unraveled by Computational Chemistry. Current Organic Chemistry, 2010, 14, 1600-1611.	0.9	6
80	Molecular Modelling of the H₂â€Adsorptive Properties of Tetrazolateâ€Based Metalâ^'Organic Frameworks: From the Cluster Approach to Periodic Simulations. ChemPhysChem, 2018, 19, 1349-1357.	1.0	6
81	Ãœber die klassische Elektronenpaarâ€•und die dative Bindung hinaus: Die Spinâ€polarisierte Bindung. Angewandte Chemie, 2021, 133, 1520-1524.	1.6	6
82	Subphthalocyaninato Boron(III) Hydride: Synthesis, Structure and Reactivity. Chemistry - A European Journal, 2021, 27, 12058-12062.	1.7	6
83	Can TD-DFT predict excited states in endoperoxides?. Computational and Theoretical Chemistry, 2011, 975, 13-19.	1.1	5
84	From Very Strong to Inexistent Beâ^'Be Bonds in the Interactions of Be₂ with Ï€â€Systems. ChemPhysChem, 2020, 21, 2701-2708.	1.0	5
85	Analysis of the bonding in XH3ï£¿Cu+ (Xï£¾B, Al, Ga) complexes. International Journal of Quantum Chemistry, 2006, 106, 659-663.	1.0	4
86	Sâ€“S Bond Activation in Multiâ€Copper ÂAggregates Containing Perthiocarboxylato Ligands. European Journal of Inorganic Chemistry, 2015, 2015, 4044-4054.	1.0	4
87	Structure and stability of [C2H4N]+singlet-state cations: Comparison between DFT and high-level ab initio calculations. International Journal of Quantum Chemistry, 2003, 91, 438-445.	1.0	3
88	On the stability of non-conventional Ï€-complexes between Ni+ and toluene, phenyl-silane and phenyl-germane. Journal of Physical Organic Chemistry, 2006, 19, 495-502.	0.9	3
89	Oxygenation of the phenylhalocarbenes. Are they spin-allowed or spin-forbidden reactions?. Journal of Molecular Modeling, 2012, 18, 2813-2821.	0.8	3
90	Insight into the optical properties of meso-pentafluorophenyl(PFP)-BODIPY: An attractive platform for functionalization of BODIPY dyes. Computational and Theoretical Chemistry, 2019, 1150, 110-120.	1.1	3

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91	Spontaneous bond dissociation cascades induced by Be_n clusters (n = 2,4). Physical Chemistry Chemical Physics, 2021, 23, 6448-6454.	1.3	3
92	Molecular Identification of the Transient Species Mediating the Deactivation Dynamics of Solvated Guanosine and Deazaguanosine. Molecules, 2022, 27, 989.	1.7	3
93	2-Oxopurine Riboside: A Dual Fluorescent Analog and Photosensitizer for RNA/DNA Research. Journal of Physical Chemistry B, 2022, 126, 4483-4490.	1.2	3
94	Theoretical Survey of the Potential Energy Surfaces Associated with the N+(3P,1D) + C2H4Reactions in the Gas Phaseâ€. Journal of Physical Chemistry A, 2004, 108, 9762-9767.	1.1	2
95	Ortho-Nitrobenzaldehyde 1:1 Water Complexes. The Influence of Solute Water Interactions in the Vertical Excited Spectrum. Zeitschrift Fur Physikalische Chemie, 2008, 222, 1263-1278.	1.4	2
96	Describing ionization of small molecules with a Gaussian and B-Splines Mixed Basis (GABS). Journal of Physics: Conference Series, 2015, 635, 112110.	0.3	2
97	Merging quantum chemistry packages with B-splines for the multichannel scattering problem. Journal of Physics: Conference Series, 2015, 635, 092013.	0.3	2
98	Unveiling the photophysics of thiourea from CASPT2/CASSCF potential energy surfaces and singlet/triplet excited state molecular dynamics simulations. Computational and Theoretical Chemistry, 2019, 1151, 36-42.	1.1	2
99	Intrastrand Photolesion Formation in Thio-Substituted DNA: A Case Study Including Single-Reference and Multireference Methods. Journal of Physical Chemistry A, 2020, 124, 10422-10433.	1.1	2
100	Significant bonding rearrangements triggered by Mg4 clusters. Journal of Chemical Physics, 2021, 154, 044302.	1.2	2
101	Ca2+ Reactivity in the Gas Phase. Bonding, Catalytic Effects and Coulomb Explosions. Challenges and Advances in Computational Chemistry and Physics, 2010, , 1-33.	0.6	2
102	Disclosing the Role of C4-Oxo Substitution in the Photochemistry of DNA and RNA Pyrimidine Monomers: Formation of Photoproducts from the Vibrationally Excited Ground State. Journal of Physical Chemistry Letters, 2022, 13, 2000-2006.	2.1	2
103	The crucial role of agostic interactions in the binding of Cu+ to alkanes, silanes and germanes in the gas phase. Journal of Computational Methods in Sciences and Engineering, 2002, 2, 411-416.	0.1	1
104	New features in the ionic states of N₂O₄: Experimental and theoretical study. Journal of Physics: Conference Series, 2012, 388, 022017.	0.3	1
105	MS-CASPT2 study of the low-lying electronic excited states of di-thiosubstituted formic acid dimers. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	1
106	Can Transition Metals and Group II Mono- and Dications Discriminate between Homo- and Heterochiral XYYXâ€™ Dimers (X,Xâ€™=H,Me; Y=O,S,Se)?. Croatica Chemica Acta, 2014, 87, 481-493.	0.1	1
107	A molecular insight into the photophysics of barbituric acid, a candidate for canonical nucleobasesâ€™ ancestor. Physical Chemistry Chemical Physics, 2022, 24, 1405-1414.	1.3	1
108	Excitation of vibrational modes in the ionization of water molecule by XUV/X-ray radiation. Journal of Physics: Conference Series, 2015, 635, 112098.	0.3	0

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109	An ab initio multiconfigurational description of core hole and shake up excited states in small molecules. Journal of Physics: Conference Series, 2015, 635, 112111.	0.3	0
110	MS-CASPT2 study of the low-lying electronic excited states of di-thiosubstituted formic acid dimers. Highlights in Theoretical Chemistry, 2014, , 17-26.	0.0	0
111	Biological systems: Applications and perspectives. , 2007, , 733-828.		0