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	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
2	Molecular Identification of the Transient Species Mediating the Deactivation Dynamics of Solvated Guanosine and Deazaguanosine. Molecules, 2022, 27, 989.	1.7	3
3	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
4	The oxidation state in low-valent beryllium and magnesium compounds. Chemical Science, 2022, 13, 6583-6591.	3.7	25
5	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
6	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
7	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
8	Ãœber die klassische Elektronenpaarâ€•und die dative Bindung hinaus: Die Spinâ€polarisierte Bindung. Angewandte Chemie, 2021, 133, 1520-1524.	1.6	6
9	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
10	Spontaneous bond dissociation cascades induced by Be_n clusters (n = 2,4). Physical Chemistry Chemical Physics, 2021, 23, 6448-6454.	1.3	3
11	Theoretical investigation of a novel xylene-based light-driven unidirectional molecular motor. Journal of Chemical Physics, 2021, 154, 064111.	1.2	10
12	Multiscale Models for Light-Driven Processes. Annual Review of Physical Chemistry, 2021, 72, 489-513.	4.8	29
13	Subphthalocyaninato Boron(III) Hydride: Synthesis, Structure and Reactivity. Chemistry - A European Journal, 2021, 27, 12058-12062.	1.7	6
14	Significant bonding rearrangements triggered by Mg4 clusters. Journal of Chemical Physics, 2021, 154, 044302.	1.2	2
15	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
16	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
17	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
18	Photochemistry in the strong coupling regime: A trajectory surface hopping scheme. Journal of Computational Chemistry, 2020, 41, 2033-2044.	1.5	25

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19	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
20	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
21	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
22	Tracking the origin of photostability in purine nucleobases: the photophysics of 2-oxopurine. Physical Chemistry Chemical Physics, 2019, 21, 13467-13473.	1.3	9
23	Mesityl or Imide Acridinium Photocatalysts: Accessible Versus Inaccessible Chargeâ€Transfer States in Photoredox Catalysis. ChemPhotoChem, 2019, 3, 609-612.	1.5	8
24	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
25	Excited state dynamics of some nonsteroidal anti-inflammatory drugs: A surface-hopping investigation. Computational and Theoretical Chemistry, 2019, 1152, 20-27.	1.1	13
26	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
27	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
28	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
29	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
30	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
31	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
32	Beryllium-based fluorenes as efficient anion sponges. Physical Chemistry Chemical Physics, 2017, 19, 23052-23059.	1.3	10
33	Photophysics and Photochemistry of Canonical Nucleobasesâ€™ Thioanalogs: From Quantum Mechanical Studies to Time Resolved Experiments. Molecules, 2017, 22, 998.	1.7	57
34	Exergonic and Spontaneous Production of Radicals through Beryllium Bonds. Angewandte Chemie - International Edition, 2016, 55, 8736-8739.	7.2	22
35	Exergonic and Spontaneous Production of Radicals through Beryllium Bonds. Angewandte Chemie, 2016, 128, 8878-8881.	1.6	9
36	The origin of efficient triplet state population in sulfur-substituted nucleobases. Nature Communications, 2016, 7, 13077.	5.8	149

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37	Berylliumâ€Based Anion Sponges: Close Relatives of Proton Sponges. Chemistry - A European Journal, 2016, 22, 18322-18325.	1.7	24
38	Surface hopping investigation of benzophenone excited state dynamics. Physical Chemistry Chemical Physics, 2016, 18, 10499-10506.	1.3	28
39	Sub-laser-cycle control of coupled electronâ€“nuclear dynamics at a conical intersection. New Journal of Physics, 2015, 17, 113023.	1.2	13
40	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
41	Sâ€“S Bond Activation in Multiâ€Copper ÂAggregates Containing Perthiocarboxylato Ligands. European Journal of Inorganic Chemistry, 2015, 2015, 4044-4054.	1.0	4
42	Merging quantum chemistry packages with B-splines for the multichannel scattering problem. Journal of Physics: Conference Series, 2015, 635, 092013.	0.3	2
43	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
44	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
45	Development of a New Dual Polarity and Viscosity Probe Based on the Foldamer Concept. Organic Letters, 2015, 17, 2844-2847.	2.4	17
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	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
48	Direct Access to Axially Substituted Subphthalocyanines from Trimethylsilyl-Protected Nucleophiles. Organic Letters, 2015, 17, 4722-4725.	2.4	26
49	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
50	Interplay of radiative and nonradiative transitions in surface hopping with radiation-molecule interactions. Journal of Chemical Physics, 2014, 140, 044113.	1.2	26
51	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:mrow><mml:mi></mml:mi></mml:msup></mml:mrow></mml:math> photodynamics of azobenzene: Decoherence and solvent effects. Computational and Theoretical Chemistry, 2014, 1040-1041, 126-135.	1.1	43
52	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
53	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
54	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

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55	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
56	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
57	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
58	Dynamics of acetone photodissociation: a surface hopping study. Physical Chemistry Chemical Physics, 2013, 15, 20651.	1.3	32
59	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
60	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
61	Surface hopping trajectory simulations with spin-orbit and dynamical couplings. Journal of Chemical Physics, 2012, 137, 22A501.	1.2	122
62	New features in the ionic states of N₂O₄: Experimental and theoretical study. Journal of Physics: Conference Series, 2012, 388, 022017.	0.3	1
63	Versatile Bottomâ€up Approach to Stapled Ïâ€Conjugated Helical Scaffolds: Synthesis and Chiroptical Properties of Cyclic oâ€Phenylene Ethynylene Oligomers. Angewandte Chemie - International Edition, 2012, 51, 13036-13040.	7.2	31
64	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
65	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
66	Semiempirical Hamiltonian for Simulation of Azobenzene Photochemistry. Journal of Physical Chemistry A, 2012, 116, 98-110.	1.1	62
67	Oxygenation of the phenylhalocarbenes. Are they spin-allowed or spin-forbidden reactions?. Journal of Molecular Modeling, 2012, 18, 2813-2821.	0.8	3
68	[MLn]2+ doubly charged systems: modeling, bonding, life times and unimolecular reactivity. Physical Chemistry Chemical Physics, 2011, 13, 14848.	1.3	13
69	Ultrafast irreversible phototautomerization of o-nitrobenzaldehyde. Chemical Communications, 2011, 47, 6383.	2.2	33
70	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
71	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
72	A comparative analysis of the UV/Vis absorption spectra of nitrobenzaldehydes. Physical Chemistry Chemical Physics, 2011, 13, 4269.	1.3	17

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73	Can TD-DFT predict excited states in endoperoxides?. Computational and Theoretical Chemistry, 2011, 975, 13-19.	1.1	5
74	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
75	On the stability and lifetime of GaO2+ in the gas phase. Theoretical Chemistry Accounts, 2011, 129, 401-407.	0.5	8
76	Gradients for configuration interaction energies with spinâ€orbit coupling in a semiempirical framework. Journal of Computational Chemistry, 2011, 32, 2690-2696.	1.5	24
77	Unexpected Gas-Phase Ion Chemistry Results Unraveled by Computational Chemistry. Current Organic Chemistry, 2010, 14, 1600-1611.	0.9	6
78	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
79	Including quantum decoherence in surface hopping. Journal of Chemical Physics, 2010, 133, 134111.	1.2	309
80	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
81	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
82	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
83	Density functional theory rationalization of the substituent effects in trifluoromethyl-pyridinol derivatives. Tetrahedron, 2009, 65, 232-239.	1.0	17
84	Theoretical investigation of anthraceneâ€9,10â€endoperoxide vertical singlet and triplet excitation spectra. Journal of Computational Chemistry, 2008, 29, 1982-1991.	1.5	15
85	Identifying the low-lying electronic states of anthracene-9,10-endoperoxide. Chemical Physics Letters, 2008, 452, 67-71.	1.2	17
86	Photodynamics of azobenzene in a hindering environment. Chemical Physics, 2008, 347, 492-502.	0.9	31
87	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
88	Electronic States of o-Nitrobenzaldehyde: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 5046-5053.	1.1	30
89	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
90	Critical appraisal of the fewest switches algorithm for surface hopping. Journal of Chemical Physics, 2007, 126, 134114.	1.2	524

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91	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
92	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
93	Biological systems: Applications and perspectives. , 2007, , 733-828.		0
94	Analysis of the bonding in XH3ï£¿Cu+ (Xï£¾B, Al, Ga) complexes. International Journal of Quantum Chemistry, 2006, 106, 659-663.	1.0	4
95	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
96	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
97	An Experimental and Theoretical Investigation of Gas-Phase Reactions of Ca2+ with Glycine. Chemistry - A European Journal, 2006, 12, 6787-6796.	1.7	57
98	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
99	On the existence and lifetimes of Cu2+ complexes with water, ammonia, and hydrogen cyanide. Journal of Chemical Physics, 2005, 123, 014315.	1.2	14
100	The importance of nonconventional structures in the binding of Ni+ to ethynylsilanes and ethynylgermanes. Theoretical Chemistry Accounts, 2004, 112, 298.	0.5	10
101	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
102	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
103	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
104	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
105	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
106	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
107	Interactions between Neutral Molecules and Ca2+:â€‰ An Assessment of Theoretical Procedures. Journal of Physical Chemistry A, 2003, 107, 10456-10461.	1.1	42
108	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

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109	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
110	Molecular gradients for semiempirical CI wavefunctions with floating occupation molecular orbitals. Chemical Physics Letters, 2000, 325, 79-85.	1.2	116
111	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