Mariona Sodupe

List of Publications by Citations

204 papers	7,284 citations	48 h-index	74 g-index
214 ext. papers	7,773 ext. citations	5.3 avg, IF	5.87 L-index

#	Paper	IF	Citations
204	Silica surface features and their role in the adsorption of biomolecules: computational modeling and experiments. *Chemical Reviews*, **2013**, 113, 4216-313	68.1	414
203	Ground State of the (H2O)2+ Radical Cation: DFT versus Post-Hartree–Fock Methods. *Journal of Physical Chemistry A*, **1999**, 103, 166-170	2.8	223
202	A theoretical study of the positive and dipositive ions of M(NH3)n and M(H2O)n for M=Mg, Ca, or Sr. *Journal of Chemical Physics*, **1992**, 96, 4453-4463	3.9	199
201	Single versus Double Proton-Transfer Reactions in Watson–Crick Base Pair Radical Cations. A Theoretical Study. *Journal of the American Chemical Society*, **1998**, 120, 8159-8167	16.4	195
200	The Different Nature of Bonding in Cu+-Glycine and Cu2+-Glycine. *Journal of Physical Chemistry B*, **1999**, 103, 2310-2317	3.4	188
199	Design, selection, and characterization of thioflavin-based intercalation compounds with metal chelating properties for application in Alzheimer's disease. *Journal of the American Chemical Society* , **2009**, 131, 1436-51	16.4	179
198	Realistic Models of Hydroxylated Amorphous Silica Surfaces and MCM-41 Mesoporous Material Simulated by Large-scale Periodic B3LYP Calculations. *Advanced Materials*, **2008**, 20, 4579-4583	24	160
197	Atomic reference energies for density functional calculations. *Chemical Physics Letters*, **1997**, 265, 481-489	2.5	146
196	Theoretical Study of M+–CO2 and OM+CO Systems for First Transition Row Metal Atoms. *Journal of Physical Chemistry A*, **1997**, 101, 7854-7859	2.8	103
195	A Quantum Chemical Study of Cu2+ Interacting with Guanine–Cytosine Base Pair. Electrostatic and Oxidative Effects on Intermolecular Proton-Transfer Processes. *Journal of Physical Chemistry A*, **2004**, 108, 333-341	2.8	99
194	Theoretical study of the bonding of the first-row transition-metal positive ions to ethylene. *The Journal of Physical Chemistry*, **1992**, 96, 2118-2122		99
193	Small molecule inhibits α-synuclein aggregation, disrupts amyloid fibrils, and prevents degeneration of dopaminergic neurons. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 10481-10486	11.5	99
192	Affinity Scale for the Interaction of Amino Acids with Silica Surfaces. *Journal of Physical Chemistry C*, **2009**, 113, 5741-5750	3.8	95
191	Theoretical study of the bonding of the first- and second-row transition-metal positive ions to acetylene. *The Journal of Physical Chemistry*, **1991**, 95, 8640-8645		93
190	Coordination of Cu+ Ions to Zeolite Frameworks Strongly Enhances Their Ability To Bind NO2. An ab Initio Density Functional Study. *Journal of the American Chemical Society*, **1998**, 120, 1545-1551	16.4	89
189	Adsorption of NH(3) and H(2)O in acidic chabazite. Comparison of ONIOM approach with periodic calculations. *Journal of Physical Chemistry B*, **2005**, 109, 3539-45	3.4	88
188	Theoretical study of one and two ammonia molecules bound to the first-row transition metal ions. *The Journal of Physical Chemistry*, **1991**, 95, 10677-10681		86

187	Can Cu+-Exchanged Zeolites Store Molecular Hydrogen? An Ab-Initio Periodic Study Compared with Low-Temperature FTIR. *Journal of Physical Chemistry B*, **2004**, 108, 8278-8286	3.4	83
186	Ground and Low-Lying States of Cu2+H2O. A Difficult Case for Density Functional Methods. *Journal of Physical Chemistry A*, **2004**, 108, 6072-6078	2.8	79
185	Protonation of glycine, serine and cysteine. Conformations, proton affinities and intrinsic basicities. *Computational and Theoretical Chemistry*, **2001**, 537, 307-318		79
184	Differences in the Activation Processes of Phosphine-Containing and Grubbs-Hoveyda-Type Alkene Metathesis Catalysts. *Organometallics*, **2012**, 31, 4203-4215	3.8	77
183	DFT mechanistic study on diene metathesis catalyzed by Ru-based Grubbs-Hoveyda-type carbenes: the key role of pi-electron density delocalization in the Hoveyda ligand. *Chemistry - A European Journal*, **2010**, 16, 7331-43	4.8	77
182	Interaction of glycine with isolated hydroxyl groups at the silica surface: first principles B3LYP periodic simulation. *Langmuir*, **2006**, 22, 6593-604	4	77
181	Ab initio molecular dynamics study of the hydration of Li(+), Na(+) and K(+) in a montmorillonite model. Influence of isomorphic substitution. *Physical Chemistry Chemical Physics*, **2010**, 12, 688-97	3.6	76
180	Theoretical Study of the Ionization of Phenol-Water and Phenol-Ammonia Hydrogen-Bonded Complexes. *Journal of Physical Chemistry A*, **1997**, 101, 9142-9151	2.8	74
179	Cation-pi Interactions and oxidative effects on Cu+ and Cu2+ binding to Phe, Tyr, Trp, and His amino acids in the gas phase. Insights from first-principles calculations. *Journal of Physical Chemistry B*, **2006**, 110, 24189-99	3.4	73
178	Does silica surface catalyse peptide bond formation? New insights from first-principles calculations. *ChemPhysChem*, **2006**, 7, 157-63	3.2	70
177	Theoretical Study of the Adsorption of RNA/DNA Bases on the External Surfaces of Na+-Montmorillonite. *Journal of Physical Chemistry C*, **2009**, 113, 13741-13749	3.8	66
176	Gas-Phase Reactivity of Ni+with Glycine. *Journal of Physical Chemistry A*, **2001**, 105, 5340-5347	2.8	66
175	Aluminosilicate surfaces as promoters for peptide bond formation: an assessment of Bernal's hypothesis by ab initio methods. *Journal of the American Chemical Society*, **2007**, 129, 8333-44	16.4	64
174	Crystal structure of thioflavin-T and its binding to amyloid fibrils: insights at the molecular level. *Chemical Communications*, **2010**, 46, 1156-8	5.8	62
173	Deep-space glycine formation via Strecker-type reactions activated by ice water dust mantles. A computational approach. *Physical Chemistry Chemical Physics*, **2010**, 12, 5285-94	3.6	60
172	Structure and fragmentation of glycine, alanine, serine and cysteine radical cations. A theoretical study. *Computational and Theoretical Chemistry*, **2005**, 727, 191-197		59
171	A theoretical study of Mg(CO2)+n and Sr(CO2)+n for n = 1 and 2 and Mg2CO+2. *Chemical Physics Letters*, **1992**, 192, 185-194	2.5	59
170	Gas phase intramolecular proton transfer in cationized glycine and chlorine substituted derivatives (M-Gly, M = Na+, Mg2+, Cu+, Ni+, and Cu2+): existence of Zwitterionic structures?. *Chemistry - A European Journal*, **2000**, 6, 4393-9	4.8	57

169	Intramolecular Proton Transfer in Glycine Radical Cation. *Journal of Physical Chemistry A*, **2000**, 104, 1256-1261	2.8	56
168	Three dimensional models of Cu(2+)-A(1-16) complexes from computational approaches. *Journal of the American Chemical Society*, **2011**, 133, 15008-14	16.4	55
167	Mechanistic insights into ring-closing enyne metathesis with the second-generation Grubbs-Hoveyda catalyst: a DFT study. *Chemistry - A European Journal*, **2011**, 17, 7506-20	4.8	55
166	Effect of Counterpoise Correction on the Geometries and Vibrational Frequencies of Hydrogen Bonded Systems. *Journal of Physical Chemistry A*, **2001**, 105, 4359-4364	2.8	53
165	Computational calculations of pKa values of imidazole in Cu(II) complexes of biological relevance. *Physical Chemistry Chemical Physics*, **2011**, 13, 7852-61	3.6	51
164	Thioflavin-T excimer formation upon interaction with amyloid fibers. *Chemical Communications*, **2013**, 49, 5745-7	5.8	50
163	Solvent-assisted catalysis in the enolization of acetaldehyde radical cation. *Chemical Physics Letters*, **2001**, 334, 112-118	2.5	50
162	A Theoretical Study of the Endo/Exo Selectivity of the Diels-Alder Reaction between Cyclopropene and Butadiene. *Journal of the American Chemical Society*, **1997**, 119, 4232-4238	16.4	49
161	Cu2+/+ cation coordination to adenine--thymine base pair. Effects on intermolecular proton-transfer processes. *Journal of Physical Chemistry B*, **2008**, 112, 4817-25	3.4	49
160	Isomerization versus Fragmentation of Glycine Radical Cation in Gas Phase. *Journal of Physical Chemistry A*, **2002**, 106, 5697-5702	2.8	49
159	Determination of the structure and bond energies of nickel dioxide and copper dioxide. *The Journal of Physical Chemistry*, **1993**, 97, 856-859		49
158	A theoretical study of the spectroscopy of MgH2O+ and MgCH3OH+. *Chemical Physics Letters*, **1992**, 195, 494-499	2.5	49
157	Hydrogen Atom or Proton Transfer in Neutral and Single Positive Ions of Salicylic Acid and Related Compounds. *Journal of the American Chemical Society*, **1999**, 121, 8882-8890	16.4	48
156	Electron hole formation in acidic zeolite catalysts. *Journal of Chemical Physics*, **2004**, 121, 6034-41	3.9	47
155	Theoretical Study of the Ionization of the H2O-H2O, NH3-H2O, and FH-H2O Hydrogen-Bonded Molecules. *Journal of the American Chemical Society*, **1994**, 116, 8249-8258	16.4	47
154	Theoretical determination of the alkali-metal superoxide bond energies. *Chemical Physics Letters*, **1992**, 195, 200-206	2.5	47
153	The calculation of the vibrational frequencies of CuCO+, NiCO and CuCH3. *Chemical Physics Letters*, **1992**, 189, 266-272	2.5	45
152	H-Bond Features of Fully Hydroxylated Surfaces of Crystalline Silica Polymorphs: A Periodic B3LYP Study. *Journal of Physical Chemistry C*, **2009**, 113, 17876-17884	3.8	44

151	Coordination properties of the oxime analogue of glycine to Cu(II). *Journal of Physical Chemistry A*, **2005**, 109, 5668-76	2.8	44
150	Keto–enol Isomerization of Acetaldehyde in HZSM5. A Theoretical Study Using the ONIOM2 Method. *Journal of Physical Chemistry B*, **2002**, 106, 10220-10226	3.4	43
149	Comparison of density functional and coupled cluster methods in the study of metal–ligand systems: Sc–CO2 and Cu–NO2. *Journal of Chemical Physics*, **1996**, 105, 9966-9971	3.9	43
148	Interaction of Co+ and Co2+ with glycine. A theoretical study. *Journal of Physical Chemistry A*, **2005**, 109, 224-30	2.8	42
147	Effects of protonation on proton-transfer processes in guanine–cytosine Watson–Crick base pairs. *Theoretical Chemistry Accounts*, **2004**, 112, 318	1.9	42
146	The role of exact exchange in the description of Cu(2+)-(H(2)O)(n) (n = 1-6) complexes by means of DFT methods. *Journal of Physical Chemistry A*, **2010**, 114, 10857-63	2.8	40
145	On the Bonding in Sc-CO2. *The Journal of Physical Chemistry*, **1995**, 99, 8567-8571		40
144	Al+–ligand binding energies. *Chemical Physics Letters*, **1991**, 181, 321-326	2.5	40
143	Influence of N7 protonation on the mechanism of the N-glycosidic bond hydrolysis in 2′-deoxyguanosine. A theoretical study. *Journal of Physical Chemistry B*, **2007**, 111, 6071-7	3.4	39
142	Influence of the Side Chain in the Structure and Fragmentation of Amino Acids Radical Cations. *Journal of Chemical Theory and Computation*, **2007**, 3, 2210-20	6.4	39
141	Visible-Light Photocatalytic Intramolecular Cyclopropane Ring Expansion. *Angewandte Chemie - International Edition*, **2017**, 56, 7826-7830	16.4	37
140	How Does Silica Catalyze the Amide Bond Formation under Dry Conditions? Role of Specific Surface Silanol Pairs. *ACS Catalysis*, **2018**, 8, 4558-4568	13.1	36
139	COMPUTATIONAL STUDY OF INTERSTELLAR GLYCINE FORMATION OCCURRING AT RADICAL SURFACES OF WATER-ICE DUST PARTICLES. *Astrophysical Journal*, **2012**, 754, 24	4.7	36
138	Theoretical study of the adsorption of DNA bases on the acidic external surface of montmorillonite. *Physical Chemistry Chemical Physics*, **2012**, 14, 945-54	3.6	36
137	Cooperative effects at water-crystalline silica interfaces strengthen surface silanol hydrogen bonding. An ab initio molecular dynamics study. *Physical Chemistry Chemical Physics*, **2012**, 14, 10507-14	3.6	36
136	On the bonding of first-row transition metal cations to guanine and adenine nucleobases. *Journal of Physical Chemistry A*, **2007**, 111, 9823-9	2.8	33
135	Effects of protonation on proton transfer processes in Watson–Crick adenine–thymine base pair. *Theoretical Chemistry Accounts*, **2007**, 118, 113-121	1.9	33
134	Palladium Nanoparticles Entrapped in Heavily Fluorinated Compounds. *Chemistry of Materials*, **2006**, 18, 716-722	9.6	33

133	Theoretical study of the alkaline-earth metal superoxides BeO2 through SrO2. *The Journal of Physical Chemistry*, **1992**, 96, 9259-9264		33
132	Role of Mineral Surfaces in Prebiotic Chemical Evolution. In Silico Quantum Mechanical Studies. *Life* , **2019**, 9,	3	30
131	Metal-mediated deamination of cytosine: experiment and DFT calculations. *Angewandte Chemie - International Edition*, **2004**, 43, 5396-9	16.4	30
130	Spin-forbidden N2O dissociation in Cu□SM-5. *Chemical Physics Letters*, **2003**, 368, 242-246	2.5	30
129	Peptide bond formation activated by the interplay of Lewis and Br□sted catalysts. *Chemical Physics Letters*, **2005**, 408, 295-301	2.5	30
128	Exo/endo Selectivity of the Ring-Closing Enyne Methathesis Catalyzed by Second Generation Ru-Based Catalysts. Influence of Reactant Substituents. *ACS Catalysis*, **2013**, 3, 206-218	13.1	28
127	Is the peptide bond formation activated by Cu(2+) interactions? Insights from density functional calculations. *Journal of Physical Chemistry B*, **2007**, 111, 5740-7	3.4	28
126	Theoretical Study of the Ionization of the H2S-H2S, PH3-H2S, and ClH-H2S Hydrogen Bonded Molecules. *Journal of the American Chemical Society*, **1995**, 117, 8416-8421	16.4	28
125	A study of the ground and low-lying states of MgCH+4. *Chemical Physics Letters*, **1993**, 214, 489-494	2.5	28
124	Physisorption vs. chemisorption of probe molecules on boron nitride nanomaterials: the effect of surface curvature. *Physical Chemistry Chemical Physics*, **2013**, 15, 13190-8	3.6	27
123	Coordination properties of glycylglycine to Cu+, Ni+ and Co+. Influence of metal cation electronic configuration. *New Journal of Chemistry*, **2005**, 29, 1585	3.6	27
122	Toward Olefin Metathesis with Iron Carbene Complexes: Benefits of Tridentate □Donating Ligands. *Organometallics*, **2016**, 35, 3914-3923	3.8	27
121	3D structures and redox potentials of Cu2+-A□1-16) complexes at different pH: a computational study. *Journal of Physical Chemistry B*, **2014**, 118, 4840-50	3.4	26
120	Periodic DFT Study of Radical Species on Crystalline Silica Surfaces. *Journal of Physical Chemistry C*, **2010**, 114, 16430-16438	3.8	26
119	DFT Study on the Relative Stabilities of Substituted Ruthenacyclobutane Intermediates Involved in Olefin Cross-Metathesis Reactions and Their Interconversion Pathways. *Organometallics*, **2014**, 33, 6065-6075	3.8	25
118	DFT study on the recovery of Hoveyda-grubbs-type catalyst precursors in enyne and diene ring-closing metathesis. *Chemistry - A European Journal*, **2013**, 19, 14553-65	4.8	25
117	On the NO Decomposition by Cu□SM-5 through the ZCu(NO2)(NO) or ZCu(N2O3) Intermediates. *Journal of Physical Chemistry B*, **2002**, 106, 1372-1379	3.4	25
116	A study of the ground and low-lying states of MgC2H2+ and MgC2H4+. *Chemical Physics*, **1994**, 185, 163-171	2.3	25

115	Diels-Alder cycloadditions of electron-rich, electron-deficient, and push-pull dienes with cyclic dienophiles: high-pressure-induced reactions and theoretical calculations. *Journal of Organic Chemistry*, **1991**, 56, 4135-4141	4.2	25
114	Amide and Peptide Bond Formation: Interplay between Strained Ring Defects and Silanol Groups at Amorphous Silica Surfaces. *Journal of Physical Chemistry C*, **2016**, 120, 24817-24826	3.8	24
113	Structures and stabilities of Fe2+/3+ complexes relevant to Alzheimer disease: an ab initio study. *Journal of Physical Chemistry A*, **2011**, 115, 12523-30	2.8	24
112	Effects of ionization on N-glycylglycine peptide: influence of intramolecular hydrogen bonds. *Journal of Chemical Physics*, **2006**, 124, 154306	3.9	24
111	Effects of ionization, metal cationization and protonation on 2deoxyguanosine: changes on sugar puckering and stability of the N-glycosidic bond. *Journal of Physical Chemistry B*, **2006**, 110, 5767-72	3.4	24
110	Water-catalyzed isomerization of the glycine radical cation. From hydrogen-atom transfer to proton-transport catalysis. *Theoretical Chemistry Accounts*, **2004**, 111, 217-222	1.9	24
109	Binding of Thioflavin T and Related Probes to Polymorphic Models of Amyloid- Fibrils. *Journal of Physical Chemistry B*, **2017**, 121, 8926-8934	3.4	23
108	Hydrogen bonding and aromaticity in the guanine ytosine base pair interacting with metal cations (M = Cu+, Ca2+ and Cu2+). *Molecular Physics*, **2005**, 103, 163-173	1.7	23
107	Triplet (pi,pi) reactivity of the guanine-cytosine DNA base pair: benign deactivation versus double tautomerization via intermolecular hydrogen transfer. *Journal of the American Chemical Society*, **2004**, 126, 12770-1	16.4	23
106	Gas phase reactivity of Cu+-aromatic amino acids: An experimental and theoretical study. *International Journal of Mass Spectrometry*, **2006**, 257, 60-69	1.9	22
105	Theoretical Study of the Structure of ZCu(NO2)(NO). A Proposed Intermediate in the NOx Decomposition by Cu ZSM-5. *Journal of Physical Chemistry A*, **2000**, 104, 3225-3230	2.8	22
104	Ab initio study of the ground and low-lying states of FeH. *Journal of Chemical Physics*, **1990**, 92, 2478-2480	3.9	22
103	Interstellar H adsorption and H formation on the crystalline (010) forsterite surface: a B3LYP-D2* periodic study. *Physical Chemistry Chemical Physics*, **2014**, 16, 17447-57	3.6	21
102	Disaggregation-induced fluorescence enhancement of NIAD-4 for the optical imaging of amyloid- fibrils. *Physical Chemistry Chemical Physics*, **2015**, 17, 19718-25	3.6	21
101	Formation versus hydrolysis of the peptide bond from a quantum-mechanical viewpoint: The role of mineral surfaces and implications for the origin of life. *International Journal of Molecular Sciences*, **2009**, 10, 746-60	6.3	21
100	Canonical, Deprotonated, or Zwitterionic? A Computational Study on Amino Acid Interaction with the TiO2 (101) Anatase Surface. *Journal of Physical Chemistry C*, **2017**, 121, 14156-14165	3.8	20
99	Thioflavin-based molecular probes for application in Alzheimer disease: from in silico to in vitro models. *Metallomics*, **2015**, 7, 83-92	4.5	20
98	On the electronic structure of second generation Hoveyda Grubbs alkene metathesis precursors. *Computational and Theoretical Chemistry*, **2012**, 996, 57-67	2	20

97	Hydrogen bond vs proton transfer in HZSM5 zeolite. A theoretical study. *Journal of Physical Chemistry B*, **2005**, 109, 19301-8	3.4	20
96	Density functional cluster model study of bonding and coordination modes of CO2 on Pd(111). *Surface Science*, **1999**, 431, 208-219	1.8	20
95	Theoretical study of the bonding of NO2 to Cu and Ag. *Journal of Chemical Physics*, **1995**, 103, 9738-9743	3.9	20
94	Water Adsorption on MO (M = Ti, Ru, and Ir) Surfaces. Importance of Octahedral Distortion and Cooperative Effects. *ACS Omega*, **2019**, 4, 2989-2999	3.9	19
93	Origin of the Enhanced Interaction of Molecular Hydrogen with Extraframework Cu+ and FeO+ Cations in Zeolite Hosts. A Periodic DFT Study. *Journal of Physical Chemistry C*, **2010**, 114, 13926-13934	3.8	19
92	Chemistry of the scandium-benzyne ion in the gas phase. *Inorganic Chemistry*, **1991**, 30, 3822-3829	5.1	19
91	Dioxygen activation in the Cu-amyloid complex. *Physical Chemistry Chemical Physics*, **2015**, 17, 27270-4	3.6	18
90	Reactivity of Metal Carbenes with Olefins: Theoretical Insights on the Carbene Electronic Structure and Cyclopropanation Reaction Mechanism. *Journal of Physical Chemistry A*, **2018**, 122, 1702-1712	2.8	18
89	Do H-bond features of silica surfaces affect the H2O and NH3 adsorption? Insights from periodic B3LYP calculations. *Journal of Physical Chemistry A*, **2011**, 115, 11221-8	2.8	18
88	Binding properties of Cu(+/2+)-(glycyl)n glycine complexes (n = 1-3). *Journal of Physical Chemistry A*, **2008**, 112, 3444-53	2.8	18
87	Elucidating the 3D structures of Al(iii)-A complexes: a template free strategy based on the pre-organization hypothesis. *Chemical Science*, **2017**, 8, 5041-5049	9.4	17
86	3-Hydroxy-4-pyridinone derivatives as metal ion and amyloid binding agents. *Metallomics*, **2014**, 6, 249-62	4.5	17
85	Ab initio design of chelating ligands relevant to Alzheimer's disease: influence of metalloaromaticity. *Journal of Physical Chemistry A*, **2011**, 115, 12659-66	2.8	17
84	Modeling Cu2+-A complexes from computational approaches. *AIP Advances*, **2015**, 5, 092402	1.5	16
83	[2 + 2] Photocycloaddition of 2(5H)-furanone to unsaturated compounds. insights from first principles calculations and transient-absorption measurements. *Journal of Organic Chemistry*, **2010**, 75, 4392-401	4.2	16
82	A DFT periodic study on the interaction between O2 and cation exchanged chabazite MCHA (M = H+, Na+ or Cu+): effects in the triplet-singlet energy gap. *Physical Chemistry Chemical Physics*, **2010**, 12, 442-52	3.6	16
81	Structure, bonding, and relative stability of the ground and low-lying electronic states of CuO2. The role of exact exchange. *Journal of Physical Chemistry A*, **2009**, 113, 1308-17	2.8	16
80	Gas Phase Reactivity of Ni+ with Urea. Mass Spectrometry and Theoretical Studies. *Journal of Physical Chemistry A*, **2003**, 107, 9865-9874	2.8	16

79	The bonding in the low-lying states of MgO+2. *Chemical Physics Letters*, **1993**, 203, 215-219	2.5	16
78	Ground and low-lying states of FeH+ as derived from ab initio self-consistent field and configuration interaction calculations. *Journal of Chemical Physics*, **1989**, 90, 6436-6442	3.9	16
77	B3LYP periodic study of the physicochemical properties of the nonpolar (010) Mg-pure and fe-containing olivine surfaces. *Journal of Physical Chemistry A*, **2014**, 118, 5866-75	2.8	15
76	Structural Behaviors of Cytosine into the Hydrated Interlayer of Na+-Montmorillonite Clay. An ab Initio Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2013**, 117, 26179-26189	3.8	15
75	A Theoretical Study on PdII Complexes Containing Hemilabile Pyrazole-Derived Ligands. *European Journal of Inorganic Chemistry*, **2006**, 2006, 447-454	2.3	15
74	Gas phase dissociation energies of saturated AHn*+ radical cations and AHn neutrals (A = Li-F, Na-Cl): dehydrogenation, deprotonation, and formation of AHn-2*+ - H2 complexes. *Journal of the American Chemical Society*, **2003**, 125, 7461-9	16.4	15
73	Theoretical study of the ScCO2 -nOScCO reaction. *Computational and Theoretical Chemistry*, **1996**, 371, 79-84		15
72	When the Surface Matters: Prebiotic Peptide-Bond Formation on the TiO (101) Anatase Surface through Periodic DFT-D2 Simulations. *Chemistry - A European Journal*, **2018**, 24, 16292-16301	4.8	15
71	Relevance of silicate surface morphology in interstellar H2formation. Insights from quantum chemical calculations. *Monthly Notices of the Royal Astronomical Society*, **2015**, 453, 914-924	4.3	14
70	Gas-Phase and Microsolvated Glycine Interacting with Boron Nitride Nanotubes. A B3LYP-D2* Periodic Study. *Inorganics*, **2014**, 2, 334-350	2.9	14
69	Insights on the binding of Thioflavin derivative markers to amyloid-like fibril models from quantum chemical calculations. *Journal of Physical Chemistry B*, **2013**, 117, 6674-80	3.4	14
68	On the mechanism of the N-glycosydic bond hydrolysis of 2?-deoxyguanosine: insights from first principles calculations. *Theoretical Chemistry Accounts*, **2011**, 128, 619-626	1.9	14
67	How the site of ionisation influences side-chain fragmentation in histidine radical cation. *Chemical Physics Letters*, **2008**, 451, 276-281	2.5	14
66	The bonding in FeC5H+5. *Chemical Physics Letters*, **1993**, 207, 19-22	2.5	14
65	An AM1 and MNDO theoretical study of the Diels-Alder reaction between .beta.-angelica lactone and cyclopentadiene. *Journal of Organic Chemistry*, **1989**, 54, 2488-2490	4.2	14
64	pH-Responsive Self-Assembly of Amyloid Fibrils for Dual Hydrolase-Oxidase Reactions. *ACS Catalysis*, **2021**, 11, 595-607	13.1	14
63	Does Fe(2+) in olivine-based interstellar grains play any role in the formation of H2? Atomistic insights from DFT periodic simulations. *Chemical Communications*, **2016**, 52, 6873-6	5.8	14
62	Interaction between Ruthenium Oxide Surfaces and Water Molecules. Effect of Surface Morphology and Water Coverage. *Journal of Physical Chemistry C*, **2019**, 123, 7786-7798	3.8	14

61	Drastic Effect of the Peptide Sequence on the Copper-Binding Properties of Tripeptides and the Electrochemical Behaviour of Their Copper(II) Complexes. *Chemistry - A European Journal*, **2018**, 24, 5153-5162	4.8	14
60	Coordination properties of a metal chelator clioquinol to Zn(2+) studied by static DFT and ab initio molecular dynamics. *Physical Chemistry Chemical Physics*, **2015**, 17, 13582-9	3.6	13
59	In silico strategies for the selection of chelating compounds with potential application in metal-promoted neurodegenerative diseases. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 21-30	4.2	13
58	Pt(II) coordination to N1 of 9-methylguanine: why it facilitates binding of additional metal ions to the purine ring. *Chemistry - A European Journal*, **2011**, 17, 9970-83	4.8	13
57	O-O bond activation in H2O2 and (CH3)3C-OOH mediated by [Ni(cyclam)(CH3CN)2](ClO4)2: different mechanisms to form the same Ni(III) product?. *Dalton Transactions*, **2011**, 40, 6868-76	4.3	13
56	Gas-phase chemistry of Sc(CH3)2+ with alkenes: activation of allylic carbon-hydrogen (C-H) bonds by a d0 system and the migratory insertion of C:C bonds into scandium-methyl (Sc+-CH3) bonds. *Journal of the American Chemical Society*, **1992**, 114, 9106-9111	16.4	13
55	Formamide Adsorption at the Amorphous Silica Surface: A Combined Experimental and Computational Approach. *Life*, **2018**, 8,	3	12
54	Enhanced photocatalytic activity of gold nanoparticles driven by supramolecular host-guest chemistry. *Chemical Communications*, **2017**, 53, 2126-2129	5.8	11
53	Influence of Ligands and Oxidation State on the Reactivity of Pentacoordinated Iron Carbenes with Olefins: Metathesis versus Cyclopropanation. *Organometallics*, **2018**, 37, 1229-1241	3.8	11
52	Influence of □stacking on the N7 and O6 proton affinity of guanine. *Theoretical Chemistry Accounts*, **2009**, 123, 105-111	1.9	11
51	Basic and acidic bifunctional catalysis: application to the tautomeric equilibrium of formamide. *Chemical Physics*, **2003**, 295, 151-158	2.3	11
50	The metal-ligand binding energies for Sr(H2O)+n. *Journal of Chemical Physics*, **1991**, 95, 9422-9423	3.9	11
49	A theoretical study of the spectroscopy of SrH2O+ and SrNH+3. *Chemical Physics Letters*, **1993**, 212, 624-630	2.3	11
48	Theoretical study of the conformational preferences in the Cl4W:CH2 complex. *Organometallics*, **1989**, 8, 1837-1841	3.8	11
47	Unusual hydrogen bonds in [AH3□H3O]+ radical cations (A=C, Si, Ge, Sn and Pb)Single-electron hydrogen bond, proton-hydride hydrogen bond and formation of [H2AOH2]+□H2 complexes. *Chemical Physics Letters*, **2004**, 395, 27-32	2.5	10
46	Coordination of NO2 to Alkaline-Earth Metals. A Theoretical Study. *Journal of Physical Chemistry A*, **1998**, 102, 630-635	2.8	10
45	Coordination of NO(2) to Cu and Mg in M(NO(2))(2) Complexes. A Theoretical Study. *Inorganic Chemistry*, **1998**, 37, 4512-4517	5.1	10
44	Comment on: An ab initio study of the ionization of sodium superoxide. *Journal of Chemical Physics*, **1992**, 96, 7871-7871	3.9	10

43	Computational study on donor-acceptor optical markers for Alzheimer disease: a game of charge transfer and electron delocalization. *Physical Chemistry Chemical Physics*, **2016**, 18, 11634-43	3.6	9
42	Gas-phase proton-transport self-catalysed isomerisation of glutamine radical cation: The important role of the side-chain. *Theoretical Chemistry Accounts*, **2007**, 118, 589-595	1.9	9
41	Bent and Linear Forms of the (Oxo)bis[trichloroferrate(III)] Dianion: An Intermolecular Effect Structural, Electronic and Magnetic Properties. *European Journal of Inorganic Chemistry*, **2003**, 2003, 4187-4194	2.3	9
40	Mixed adenine/guanine quartets with three trans-a2 Pt(II) (a=NH(3) or MeNH(2)) cross-links: linkage and rotational isomerism, base pairing, and loss of NH(3). *Chemistry - A European Journal*, **2014**, 20, 3394-407	4.8	8
39	In silico study of the interstellar prebiotic formation and delivery of glycine. *Rendiconti Lincei*, **2011**, 22, 137-144	1.7	8
38	Coordination of (glycyl)(n)glycine (n = 1-3) to Co+ and Co2+. *Journal of Physical Chemistry A*, **2009**, 113, 8883-92	2.8	8
37	Coordination properties of lysine interacting with Co(I) and Co(II). A theoretical and mass spectrometry study. *Journal of Physical Chemistry A*, **2008**, 112, 12385-92	2.8	8
36	What is the structure of FeC5H6+?. *Chemical Physics Letters*, **1995**, 240, 526-532	2.5	8
35	Theoretical study of the 2A2?2B2 separation of the alkali superoxides. *Chemical Physics Letters*, **1992**, 197, 213-216	2.5	8
34	Fluorous l-Carbidopa Precursors: Highly Enantioselective Synthesis and Computational Prediction of Bioactivity. *Journal of Organic Chemistry*, **2018**, 83, 303-313	4.2	8
33	Strained ring motif at silica surfaces: A quantum mechanical study of their reactivity towards protic molecules. *Computational and Theoretical Chemistry*, **2015**, 1074, 168-177	2	7
32	BCN-M: A Free Computational Tool for Generating Wulff-like Nanoparticle Models with Controlled Stoichiometry. *Journal of Physical Chemistry C*, **2020**, 124, 1227-1237	3.8	7
31	Multiple Condensation Reactions Involving Pt(II) /Pd(II) -OH2 , Pt-NH3 , and Cytosine-NH2 Groups: New Twists in Cisplatin-Nucleobase Chemistry. *Chemistry - A European Journal*, **2016**, 22, 13653-68	4.8	6
30	Stability of transient Cu+A(1?16) species and influence of coordination and peptide configuration on superoxide formation. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	6
29	Surface Reaction of Acetylene with H-Terminated Silicon Surfaces. A Theoretical Study from Hybrid DFT-D2 Periodic Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 15130-15138	3.8	6
28	Influence of ionization on the conformational preferences of peptide models. Ramachandran surfaces of N-formyl-glycine amide and N-formyl-alanine amide radical cations. *Journal of Computational Chemistry*, **2009**, 30, 1771-84	3.5	6
27	Mechanismus der metallvermittelten Desaminierung von Cytosin Experiment und DFT-Rechnungen. *Angewandte Chemie*, **2004**, 116, 5507-5511	3.6	6
26	Hydrogen Bonding and Proton Transfer in ionized DNA Base Pairs, Amino Acids and Peptides **2010**, 219-243		5

25	Ab initio study of the reaction between Cl4W?CH2 and ethylene. *Computational and Theoretical Chemistry*, **1991**, 251, 37-47		5
24	Activating a Peroxo Ligand for C-O Bond Formation. *Angewandte Chemie - International Edition*, **2019**, 58, 3037-3041	16.4	5
23	Canonical Watson□Crick base pair interactions in □-π type triplet states. *Molecular Physics*, **2006**, 104, 925-931	1.7	4
22	Unusual hydrogen bonds in [AH3□H3O]+ radical cations (A = C, Si, Ge, Sn and Pb): Single-electron hydrogen bond, proton-hydride hydrogen bond and formation of [H2AOH2]+□H2 complexes. *Chemical Physics Letters*, **2004**, 395, 27-32	2.5	4
21	Enhanced Metallophilicity in Metal-Carbene Systems: Stronger Character of Aurophilic Interactions in Solution. *Chemistry - A European Journal*, **2020**, 26, 997-1002	4.8	4
20	Aerobic intramolecular carbon-hydrogen bond oxidation promoted by Cu(I) complexes. *Dalton Transactions*, **2020**, 49, 14647-14655	4.3	4
19	Nucleobase Stacking at Clay Edges, a Favorable Interaction for RNA/DNA Oligomerization. *ACS Earth and Space Chemistry*, **2019**, 3, 1023-1033	3.2	3
18	Theoretical study of ScCO2+. *International Journal of Quantum Chemistry*, **1997**, 63, 523-528	2.1	3
17	Importance of the oxyl character on the IrO2 surface dependent catalytic activity for the oxygen evolution reaction. *Journal of Catalysis*, **2021**, 396, 192-201	7.3	3
16	Site-selective-induced isomerization of formamide. *Physical Chemistry Chemical Physics*, **2019**, 21, 25626-25634	3.6	3
15	Atomistic fibrillar architectures of polar prion-inspired heptapeptides. *Chemical Science*, **2020**, 11, 13143-13151	9.4	2
14	Intramolecular Photocycloaddition of 2(5 H)-Furanones to Temporarily Tethered Terminal Alkenes as a Stereoselective Source of Enantiomerically Pure Polyfunctionalyzed Cyclobutanes. *Journal of Organic Chemistry*, **2018**, 83, 3188-3199	4.2	2
13	Theoretical study of the bonding of the first-row transition-metal positive ions to ethylene. [Erratum to document cited in CA116(13):128993g]. *The Journal of Physical Chemistry*, **1992**, 96, 5670-5670		2
12	The role of charge transfer in the photophysics of dithiophene-based (NIADs) fluorescent markers for amyloid-□detection. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	2
11	Activating a Peroxo Ligand for C□O Bond Formation. *Angewandte Chemie*, **2019**, 131, 3069-3073	3.6	2
10	Fluorescent Markers for Amyloid-□Detection: Computational Insights. *Israel Journal of Chemistry*, **2017**, 57, 686-698	3.4	1
9	An ab initio study of the collinear reaction of Fe+ (4F) and Fe+ (6D) with H2. *Journal of Chemical Physics*, **1991**, 94, 4352-4355	3.9	1
8	First-Principles Modeling of Protein/Surface Interactions. Polyglycine Secondary Structure Adsorption on the TiO (101) Anatase Surface Adopting a Full Periodic Approach. *Journal of Chemical Information and Modeling*, **2021**, 61, 5484-5498	6.1	1

List of Publications

7	Impact of Cu(II) and Al(III) on the conformational landscape of amyloid *Physical Chemistry Chemical Physics*, **2021**, 23, 13023-13032	3.6	1
6	Surface morphology controls water dissociation on hydrated IrO nanoparticles. *Nanoscale*, **2021**, 13, 14480-14489	7.7	0
5	Computational Simulations of Prebiotic Processes. *Cellular Origin and Life in Extreme Habitats*, **2012**, 345-362		
4	Theoretical and computational chemistry in Spain. *Theoretical Chemistry Accounts*, **2011**, 128, 389-391	1.9	
3	Effects of Ionization and Cationization on Intermolecular Proton Transfer Reactions in DNA base Pairs **2003**, 1231-1255		
2	Formamide Dehydration and Condensation on Acidic Montmorillonite: Mechanistic Insights from Ab-Initio Periodic Simulations. *Lecture Notes in Computer Science*, **2020**, 502-512	0.9	
1	Atomistic insights into the structure of heptapeptide nanofibers. *Journal of Chemical Physics*, **2021**, 155, 055101	3.9	