Mariona Sodupe

List of Publications by Year
in descending order

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209 papers	8,290 citations	41339 49 h-index	64791 79 g-index
214 all docs	214 docs citations	214 times ranked	7124 citing authors

#	Article	IF	Citations
1	Silica Surface Features and Their Role in the Adsorption of Biomolecules: Computational Modeling and Experiments. Chemical Reviews, 2013, 113, 4216-4313.	47.7	508
2	Ground State of the (H2O)2+ Radical Cation:â€‰ DFT versus Post-Hartreeâ^'Fock Methods. Journal of Physical Chemistry A, 1999, 103, 166-170.	2.5	232
3	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.	3.0	206
4	Single versus Double Proton-Transfer Reactions in Watsonâ^'Crick Base Pair Radical Cations. A Theoretical Study. Journal of the American Chemical Society, 1998, 120, 8159-8167.	13.7	203
5	Realistic Models of Hydroxylated Amorphous Silica Surfaces and MCMâ€41 Mesoporous Material Simulated by Largeâ€scale Periodic B3LYP Calculations. Advanced Materials, 2008, 20, 4579-4583.	21.0	199
6	The Different Nature of Bonding in Cu+-Glycine and Cu2+-Glycine. Journal of Physical Chemistry B, 1999, 103, 2310-2317.	2.6	198
7	Design, Selection, and Characterization of Thioflavin-Based Intercalation Compounds with Metal Chelating Properties for Application in Alzheimerâ€™s Disease. Journal of the American Chemical Society, 2009, 131, 1436-1451.	13.7	196
8	Small molecule inhibits Î±-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.	7.1	166
9	Atomic reference energies for density functional calculations. Chemical Physics Letters, 1997, 265, 481-489.	2.6	154
10	Theoretical Study of M+â^'CO2and OM+CO Systems for First Transition Row Metal Atoms. Journal of Physical Chemistry A, 1997, 101, 7854-7859.	2.5	112
11	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.	13.7	109
12	A Quantum Chemical Study of Cu2+ Interacting with Guanineâ^'Cytosine Base Pair. Electrostatic and Oxidative Effects on Intermolecular Proton-Transfer Processes. Journal of Physical Chemistry A, 2004, 108, 333-341.	2.5	106
13	Affinity Scale for the Interaction of Amino Acids with Silica Surfaces. Journal of Physical Chemistry C, 2009, 113, 5741-5750.	3.1	105
14	Theoretical study of the bonding of the first-row transition-metal positive ions to ethylene. The Journal of Physical Chemistry, 1992, 96, 2118-2122.	2.9	101
15	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.	2.9	100
16	Adsorption of NH3and H2O in Acidic Chabazite. Comparison of ONIOM Approach with Periodic Calculations. Journal of Physical Chemistry B, 2005, 109, 3539-3545.	2.6	96
17	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.	2.6	91
18	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.	2.9	90

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19	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, 688-697.	2.8	90
20	Ground and Low-Lying States of Cu2+â^'H2O. A Difficult Case for Density Functional Methods. Journal of Physical Chemistry A, 2004, 108, 6072-6078.	2.5	85
21	Differences in the Activation Processes of Phosphine-Containing and Grubbsâ€"Hoveyda-Type Alkene Metathesis Catalysts. Organometallics, 2012, 31, 4203-4215.	2.3	85
22	Protonation of glycine, serine and cysteine. Conformations, proton affinities and intrinsic basicities. Computational and Theoretical Chemistry, 2001, 537, 307-318.	1.5	83
23	Interaction of Glycine with Isolated Hydroxyl Groups at the Silica Surface:â€‰ First Principles B3LYP Periodic Simulation. Langmuir, 2006, 22, 6593-6604.	3.5	83
24	DFT Mechanistic Study on Diene Metathesis Catalyzed by Ruâ€Based Grubbsâ€"Hoveydaâ€Type Carbenes: The Key Role of Ï€â€Electron Density Delocalization in the Hoveyda Ligand. Chemistry - A European Journal, 2010, 16, 7331-7343.	3.3	78
25	Crystal structure of thioflavin-T and its binding to amyloid fibrils: insights at the molecular level. Chemical Communications, 2010, 46, 1156.	4.1	78
26	Cationâ^'Ï€ 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, 24189-24199.	2.6	77
27	Does Silica Surface Catalyse Peptide Bond Formation? New Insights from First-Principles Calculations. ChemPhysChem, 2006, 7, 157-163.	2.1	77
28	Deep-space glycine formation via Strecker-type reactions activated by ice water dust mantles. A computational approach. Physical Chemistry Chemical Physics, 2010, 12, 5285.	2.8	77
29	Theoretical Study of the Ionization of Phenolâ^'Water and Phenolâ^'Ammonia Hydrogen-Bonded Complexes. Journal of Physical Chemistry A, 1997, 101, 9142-9151.	2.5	76
30	Aluminosilicate Surfaces as Promoters for Peptide Bond Formation:Â An Assessment of Bernal's Hypothesis by ab Initio Methods. Journal of the American Chemical Society, 2007, 129, 8333-8344.	13.7	75
31	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.	3.1	72
32	Gas-Phase Reactivity of Ni+with Glycine. Journal of Physical Chemistry A, 2001, 105, 5340-5347.	2.5	66
33	Structure and fragmentation of glycine, alanine, serine and cysteine radical cations. A theoretical study. Computational and Theoretical Chemistry, 2005, 727, 191-197.	1.5	63
34	Three Dimensional Models of Cu²⁺-AÎ²(1â€"16) Complexes from Computational Approaches. Journal of the American Chemical Society, 2011, 133, 15008-15014.	13.7	61
35	Gas Phase Intramolecular Proton Transfer in Cationized Glycine and Chlorine Substituted Derivatives (Mâ€"Gly, M=Na+, Mg2+, Cu+, Ni+, and Cu2+): Existence of Zwitterionic Structures?. Chemistry - A European Journal, 2000, 6, 4393-4399.	3.3	60
36	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.	2.6	59

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37	Intramolecular Proton Transfer in Glycine Radical Cation. Journal of Physical Chemistry A, 2000, 104, 1256-1261.	2.5	59
38	Effect of Counterpoise Correction on the Geometries and Vibrational Frequencies of Hydrogen Bonded Systems. Journal of Physical Chemistry A, 2001, 105, 4359-4364.	2.5	57
39	Mechanistic Insights into Ringâ€Closing Enyne Metathesis with the Secondâ€Generation Grubbsâ€“Hoveyda Catalyst: A DFT Study. Chemistry - A European Journal, 2011, 17, 7506-7520.	3.3	56
40	Thioflavin-T excimer formation upon interaction with amyloid fibers. Chemical Communications, 2013, 49, 5745.	4.1	56
41	A Theoretical Study of the Endo/Exo Selectivity of the Dielsâ^'Alder Reaction between Cyclopropene and Butadiene. Journal of the American Chemical Society, 1997, 119, 4232-4238.	13.7	55
42	Computational calculations of pKa values of imidazole in Cu(ii) complexes of biological relevance. Physical Chemistry Chemical Physics, 2011, 13, 7852.	2.8	55
43	H-Bond Features of Fully Hydroxylated Surfaces of Crystalline Silica Polymorphs: A Periodic B3LYP Study. Journal of Physical Chemistry C, 2009, 113, 17876-17884.	3.1	54
44	Determination of the structure and bond energies of nickel dioxide and copper dioxide. The Journal of Physical Chemistry, 1993, 97, 856-859.	2.9	53
45	Solvent-assisted catalysis in the enolization of acetaldehyde radical cation. Chemical Physics Letters, 2001, 334, 112-118.	2.6	52
46	Cu^{2+/+} Cation Coordination to Adenineâ^'Thymine Base Pair. Effects on Intermolecular Proton-Transfer Processes. Journal of Physical Chemistry B, 2008, 112, 4817-4825.	2.6	52
47	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.	13.7	51
48	COMPUTATIONAL STUDY OF INTERSTELLAR GLYCINE FORMATION OCCURRING AT RADICAL SURFACES OF WATER-ICE DUST PARTICLES. Astrophysical Journal, 2012, 754, 24.	4.5	51
49	How Does Silica Catalyze the Amide Bond Formation under Dry Conditions? Role of Specific Surface Silanol Pairs. ACS Catalysis, 2018, 8, 4558-4568.	11.2	51
50	A theoretical study of the spectroscopy of MgH2O+ and MgCH3OH+. Chemical Physics Letters, 1992, 195, 494-499.	2.6	50
51	The calculation of the vibrational frequencies of CuCO+, NiCO and CuCH3. Chemical Physics Letters, 1992, 189, 266-272.	2.6	49
52	Isomerization versus Fragmentation of Glycine Radical Cation in Gas Phase. Journal of Physical Chemistry A, 2002, 106, 5697-5702.	2.5	49
53	Electron hole formation in acidic zeolite catalysts. Journal of Chemical Physics, 2004, 121, 6034-6041.	3.0	49
54	pH-Responsive Self-Assembly of Amyloid Fibrils for Dual Hydrolase-Oxidase Reactions. ACS Catalysis, 2021, 11, 595-607.	11.2	49

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55	Theoretical determination of the alkali-metal superoxide bond energies. Chemical Physics Letters, 1992, 195, 200-206.	2.6	48
56	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.	13.7	48
57	Effects of protonation on proton-transfer processes in guanine?cytosine Watson?Crick base pairs. Theoretical Chemistry Accounts, 2004, 112, 318.	1.4	48
58	Visibleâ€Light Photocatalytic Intramolecular Cyclopropane Ring Expansion. Angewandte Chemie - International Edition, 2017, 56, 7826-7830.	13.8	47
59	Comparison of density functional and coupled cluster methods in the study of metalâ€“ligand systems: Scâ€“CO2 and Cuâ€“NO2. Journal of Chemical Physics, 1996, 105, 9966-9971.	3.0	46
60	Ketoâ^'Enol Isomerization of Acetaldehyde in HZSM5. A Theoretical Study Using the ONIOM2 Method. Journal of Physical Chemistry B, 2002, 106, 10220-10226.	2.6	46
61	Coordination Properties of the Oxime Analogue of Glycine to Cu(II). Journal of Physical Chemistry A, 2005, 109, 5668-5676.	2.5	46
62	Role of Mineral Surfaces in Prebiotic Chemical Evolution. In Silico Quantum Mechanical Studies. Life, 2019, 9, 10.	2.4	44
63	The Role of Exact Exchange in the Description of Cu²⁺â^'(H₂O)_n(n= 1â^'6) Complexes by Means of DFT Methods. Journal of Physical Chemistry A, 2010, 114, 10857-10863.	2.5	43
64	Cooperative effects at waterâ€“crystalline silica interfaces strengthen surface silanol hydrogen bonding. An ab initio molecular dynamics study. Physical Chemistry Chemical Physics, 2012, 14, 10507.	2.8	43
65	Al+â€”ligand binding energies. Chemical Physics Letters, 1991, 181, 321-326.	2.6	42
66	Interaction of Co+ and Co2+ with Glycine. A Theoretical Study. Journal of Physical Chemistry A, 2005, 109, 224-230.	2.5	42
67	Influence of N7 Protonation on the Mechanism of the N-Glycosidic Bond Hydrolysis in 2â€˜-Deoxyguanosine. A Theoretical Study. Journal of Physical Chemistry B, 2007, 111, 6071-6077.	2.6	42
68	On the Bonding in Sc-CO2. The Journal of Physical Chemistry, 1995, 99, 8567-8571.	2.9	41
69	Influence of the Side Chain in the Structure and Fragmentation of Amino Acids Radical Cations. Journal of Chemical Theory and Computation, 2007, 3, 2210-2220.	5.3	41
70	Theoretical study of the adsorption of DNA bases on the acidic external surface of montmorillonite. Physical Chemistry Chemical Physics, 2012, 14, 945-954.	2.8	39
71	Palladium Nanoparticles Entrapped in Heavily Fluorinated Compounds. Chemistry of Materials, 2006, 18, 716-722.	6.7	38
72	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.	3.2	37

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73	Effects of protonation on proton transfer processes in Watsonâ€“Crick adenineâ€“thymine base pair. Theoretical Chemistry Accounts, 2007, 118, 113-121.	1.4	36
74	Theoretical study of the alkaline-earth metal superoxides BeO2 through SrO2. The Journal of Physical Chemistry, 1992, 96, 9259-9264.	2.9	35
75	Peptide bond formation activated by the interplay of Lewis and BrÃ¸nsted catalysts. Chemical Physics Letters, 2005, 408, 295-301.	2.6	35
76	On the Bonding of First-Row Transition Metal Cations to Guanine and Adenine Nucleobases. Journal of Physical Chemistry A, 2007, 111, 9823-9829.	2.5	34
77	Binding of Thioflavin T and Related Probes to Polymorphic Models of Amyloid-Î² Fibrils. Journal of Physical Chemistry B, 2017, 121, 8926-8934.	2.6	34
78	Metal-Mediated Deamination of Cytosine: Experiment and DFT Calculations. Angewandte Chemie - International Edition, 2004, 43, 5396-5399.	13.8	33
79	Coordination properties of glycylglycine to Cu+, Ni+ and Co+. Influence of metal cation electronic configuration. New Journal of Chemistry, 2005, 29, 1585.	2.8	32
80	Hydrogen bonding and aromaticity in the guanineâ€“cytosine base pair interacting with metal cations (Mâ€‰=â€‰Cu+, Ca2+and Cu2+). Molecular Physics, 2005, 103, 163-173.	1.7	32
81	Is the Peptide Bond Formation Activated by Cu2+Interactions? Insights from Density Functional Calculations. Journal of Physical Chemistry B, 2007, 111, 5740-5747.	2.6	32
82	Toward Olefin Metathesis with Iron Carbene Complexes: Benefits of Tridentate Ïƒ-Donating Ligands. Organometallics, 2016, 35, 3914-3923.	2.3	32
83	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.	11.2	31
84	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.	2.3	31
85	Spin-forbidden N2O dissociation in Cuâ€“ZSM-5. Chemical Physics Letters, 2003, 368, 242-246.	2.6	30
86	Physisorption vs. chemisorption of probe molecules on boron nitride nanomaterials: the effect of surface curvature. Physical Chemistry Chemical Physics, 2013, 15, 13190.	2.8	30
87	DFT Study on the Recovery of Hoveydaâ€“Grubbsâ€Type Catalyst Precursors in Enyne and Diene Ringâ€Closing Metathesis. Chemistry - A European Journal, 2013, 19, 14553-14565.	3.3	30
88	3D Structures and Redox Potentials of Cu²⁺â€“AÎ²(1â€“16) Complexes at Different pH: A Computational Study. Journal of Physical Chemistry B, 2014, 118, 4840-4850.	2.6	30
89	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.	3.1	30
90	A study of the ground and low-lying states of MgCH+4. Chemical Physics Letters, 1993, 214, 489-494.	2.6	28

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91	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.	13.7	28
92	Interstellar H adsorption and H₂formation on the crystalline (010) forsterite surface: a B3LYP-D2* periodic study. Physical Chemistry Chemical Physics, 2014, 16, 17447-17457.	2.8	28
93	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.	3.1	28
94	Water Adsorption on MO₂ (M = Ti, Ru, and Ir) Surfaces. Importance of Octahedral Distortion and Cooperative Effects. ACS Omega, 2019, 4, 2989-2999.	3.5	28
95	Periodic DFT Study of Radical Species on Crystalline Silica Surfaces. Journal of Physical Chemistry C, 2010, 114, 16430-16438.	3.1	27
96	Structures and Stabilities of Fe2+/3+Complexes Relevant to Alzheimerâ€™s Disease: An ab Initio Study. Journal of Physical Chemistry A, 2011, 115, 12523-12530.	2.5	27
97	Water-catalyzed isomerization of the glycine radical cation. From hydrogen-atom transfer to proton-transport catalysis. Theoretical Chemistry Accounts, 2004, 111, 217-222.	1.4	26
98	Effects of ionization on N-glycylglycine peptide: Influence of intramolecular hydrogen bonds. Journal of Chemical Physics, 2006, 124, 154306.	3.0	26
99	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.	2.5	26
100	A study of the ground and low-lying states of MgC2H2+ and MgC2H4+. Chemical Physics, 1994, 185, 163-171.	1.9	25
101	Theoretical Study of the Structure of ZCu(NO2)(NO). A Proposed Intermediate in the NOx Decomposition by Cuâ^'ZSM-5. Journal of Physical Chemistry A, 2000, 104, 3225-3230.	2.5	25
102	On the NO Decomposition by Cuâ^'ZSM-5 through the ZCu(NO2)(NO) or ZCu(N2O3) Intermediates. Journal of Physical Chemistry B, 2002, 106, 1372-1379.	2.6	25
103	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, 11221-11228.	2.5	25
104	Ab initio study of the ground and lowâ€lying states of FeH. Journal of Chemical Physics, 1990, 92, 2478-2480.	3.0	24
105	Effects of Ionization, Metal Cationization and Protonation on 2â€˜-Deoxyguanosine:Â Changes on Sugar Puckering and Stability of the N-Glycosidic Bond. Journal of Physical Chemistry B, 2006, 110, 5767-5772.	2.6	24
106	Gas phase reactivity of Cu+-aromatic amino acids. International Journal of Mass Spectrometry, 2006, 257, 60-69.	1.5	24
107	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, 746-760.	4.1	24
108	Disaggregation-induced fluorescence enhancement of NIAD-4 for the optical imaging of amyloid-Î² fibrils. Physical Chemistry Chemical Physics, 2015, 17, 19718-19725.	2.8	24

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109	Dioxygen activation in the Cuâ€“amyloid Î² complex. Physical Chemistry Chemical Physics, 2015, 17, 27270-27274.	2.8	24
110	Drastic Effect of the Peptide Sequence on the Copperâ€Binding Properties of Tripeptides and the Electrochemical Behaviour of Their Copper(II) Complexes. Chemistry - A European Journal, 2018, 24, 5153-5162.	3.3	24
111	Triplet (Ï€,Ï€*) Reactivity of the Guanineâ‹¯Cytosine DNA Base Pair:Â Benign Deactivation versus Double Tautomerization via Intermolecular Hydrogen Transfer. Journal of the American Chemical Society, 2004, 126, 12770-12771.	13.7	23
112	Relevance of silicate surface morphology in interstellar H₂formation. Insights from quantum chemical calculations. Monthly Notices of the Royal Astronomical Society, 2015, 453, 914-924.	4.4	23
113	Thioflavin-based molecular probes for application in Alzheimer's disease: from in silico to in vitro models. Metallomics, 2015, 7, 83-92.	2.4	23
114	When the Surface Matters: Prebiotic Peptideâ€Bond Formation on the TiO₂ (101) Anatase Surface through Periodic DFTâ€D2 Simulations. Chemistry - A European Journal, 2018, 24, 16292-16301.	3.3	23
115	Chemistry of the scandium-benzyne ion in the gas phase. Inorganic Chemistry, 1991, 30, 3822-3829.	4.0	22
116	Hydrogen Bond vs Proton Transfer in HZSM5 Zeolite. A Theoretical Study. Journal of Physical Chemistry B, 2005, 109, 19301-19308.	2.6	22
117	Does Fe²⁺ in olivine-based interstellar grains play any role in the formation of H₂? Atomistic insights from DFT periodic simulations. Chemical Communications, 2016, 52, 6873-6876.	4.1	22
118	Theoretical study of the bonding of NO2 to Cu and Ag. Journal of Chemical Physics, 1995, 103, 9738-9743.	3.0	21
119	Density functional cluster model study of bonding and coordination modes of CO2 on Pd(111). Surface Science, 1999, 431, 208-219.	1.9	21
120	On the electronic structure of second generation Hoveydaâ€“Grubbs alkene metathesis precursors. Computational and Theoretical Chemistry, 2012, 996, 57-67.	2.5	21
121	Elucidating the 3D structures of Al(<scp>iii</scp>)â€“AÎ² complexes: a template free strategy based on the pre-organization hypothesis. Chemical Science, 2017, 8, 5041-5049.	7.4	21
122	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.	3.1	20
123	Ab Initio Design of Chelating Ligands Relevant to Alzheimerâ€™s Disease: Influence of Metalloaromaticity. Journal of Physical Chemistry A, 2011, 115, 12659-12666.	2.5	20
124	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, 5866-5875.	2.5	20
125	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.	3.0	19
126	Binding Properties of Cu^{+/2+}-(glycyl)_nglycine Complexes (n =) Tj ETQq0 0 0 rgBT /Overlock 10 T	2.5	19

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127	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, 1308-1317.	2.5	19
128	A DFT periodic study on the interaction between O₂and cation exchanged chabazite MCHA (M = H+, Na+ or Cu+): effects in the tripletâ€“singlet energy gap. Physical Chemistry Chemical Physics, 2010, 12, 442-452.	2.8	19
129	Insights on the Binding of Thioflavin Derivative Markers to Amyloid-Like Fibril Models from Quantum Chemical Calculations. Journal of Physical Chemistry B, 2013, 117, 6674-6680.	2.6	19
130	3-Hydroxy-4-pyridinone derivatives as metal ion and amyloid binding agents. Metallomics, 2014, 6, 249-262.	2.4	19
131	Gas Phase Dissociation Energies of Saturated AHnÂ·+Radical Cations and AHnNeutrals (A = Liâ^'F, Naâ^'Cl):Â Dehydrogenation, Deprotonation, and Formation of AHn-2Â·+ÂÂ â^' H2Complexes. Journal of the American Chemical Society, 2003, 125, 7461-7469.	13.7	18
132	Gas Phase Reactivity of Ni+ with Urea. Mass Spectrometry and Theoretical Studies. Journal of Physical Chemistry A, 2003, 107, 9865-9874.	2.5	18
133	A Theoretical Study on PdII Complexes Containing Hemilabile Pyrazole-Derived Ligands. European Journal of Inorganic Chemistry, 2006, 2006, 447-454.	2.0	18
134	Interaction between Ruthenium Oxide Surfaces and Water Molecules. Effect of Surface Morphology and Water Coverage. Journal of Physical Chemistry C, 2019, 123, 7786-7798.	3.1	18
135	Importance of the oxyl character on the IrO2 surface dependent catalytic activity for the oxygen evolution reaction. Journal of Catalysis, 2021, 396, 192-201.	6.2	18
136	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.	3.2	17
137	[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, 4392-4401.	3.2	17
138	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.	3.1	17
139	Modeling Cu2+-Aβ2 complexes from computational approaches. AIP Advances, 2015, 5, 092402.	1.3	17
140	Theoretical study of the conformational preferences in the Cl4W:CH2 complex. Organometallics, 1989, 8, 1837-1841.	2.3	16
141	The bonding in the low-lying states of MgO+2. Chemical Physics Letters, 1993, 203, 215-219.	2.6	16
142	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.	13.7	15
143	Theoretical study of the ScCO2 â†' OScCO reaction. Computational and Theoretical Chemistry, 1996, 371, 79-84.	1.5	15
144	Oâ€“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.	3.3	15

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145	Gas-Phase and Microsolvated Glycine Interacting with Boron Nitride Nanotubes. A B3LYP-D2* Periodic Study. Inorganics, 2014, 2, 334-350.	2.7	15
146	The bonding in FeC5H+5. Chemical Physics Letters, 1993, 207, 19-22.	2.6	14
147	How the site of ionisation influences side-chain fragmentation in histidine radical cation. Chemical Physics Letters, 2008, 451, 276-281.	2.6	14
148	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.	2.9	14
149	On the mechanism of the N-glycosydic bond hydrolysis of 2â€²-deoxyguanosine: insights from first principles calculations. Theoretical Chemistry Accounts, 2011, 128, 619-626.	1.4	14
150	Pt^{II} Coordination to N1 of 9â€Methylguanine: Why it Facilitates Binding of Additional Metal Ions to the Purine Ring. Chemistry - A European Journal, 2011, 17, 9970-9983.	3.3	14
151	Influence of Ligands and Oxidation State on the Reactivity of Pentacoordinated Iron Carbenes with Olefins: Metathesis versus Cyclopropanation. Organometallics, 2018, 37, 1229-1241.	2.3	14
152	Formamide Adsorption at the Amorphous Silica Surface: A Combined Experimental and Computational Approach. Life, 2018, 8, 42.	2.4	14
153	Prebiotic chemistry. Chemical Society Reviews, 2012, 41, 5373.	38.1	13
154	Coordination properties of a metal chelator clioquinol to Zn²⁺ studied by static DFT and ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2015, 17, 13582-13589.	2.8	13
155	BCN-M: A Free Computational Tool for Generating Wulff-like Nanoparticle Models with Controlled Stoichiometry. Journal of Physical Chemistry C, 2020, 124, 1227-1237.	3.1	13
156	Metal coordination determines the catalytic activity of IrO2 nanoparticles for the oxygen evolution reaction. Journal of Catalysis, 2022, 412, 78-86.	6.2	13
157	Basic and acidic bifunctional catalysis: application to the tautomeric equilibrium of formamide. Chemical Physics, 2003, 295, 151-158.	1.9	12
158	Unusual hydrogen bonds in [AH3â€“H3O]+ radical cations (A=C, Si, Ge, Sn and Pb)Single-electron hydrogen bond, proton-hydride hydrogen bond and formation of [H2AOH2]+â€“H2 complexes. Chemical Physics Letters, 2004, 395, 27-32.	2.6	12
159	The metalâ€ligand binding energies for Sr(H2O)+n. Journal of Chemical Physics, 1991, 95, 9422-9423.	3.0	11
160	Comment on: Anabinitiostudy of the ionization of sodium superoxide. Journal of Chemical Physics, 1992, 96, 7871-7871.	3.0	11
161	A theoretical study of the spectroscopy of SrH2O+ and SrNH+3. Chemical Physics Letters, 1993, 212, 624-630.	2.6	11
162	Coordination of NO2to Cu and Mg in M(NO2)2Complexes. A Theoretical Study. Inorganic Chemistry, 1998, 37, 4512-4517.	4.0	11

#	Article	IF	Citations
163	Influence of Ï€-stacking on the N7 and O6 proton affinity of guanine. Theoretical Chemistry Accounts, 2009, 123, 105-111.	1.4	11
164	Enhanced photocatalytic activity of gold nanoparticles driven by supramolecular hostâ€“guest chemistry. Chemical Communications, 2017, 53, 2126-2129.	4.1	11
165	Enhanced Metallophilicity in Metalâ€“Carbene Systems: Stronger Character of Aurophilic Interactions in Solution. Chemistry - A European Journal, 2020, 26, 997-1002.	3.3	11
166	Coordination of NO2to Alkaline-Earth Metals. A Theoretical Study. Journal of Physical Chemistry A, 1998, 102, 630-635.	2.5	10
167	Bent and Linear Forms of the (Î¼-Oxo)bis[trichloroferrate(III)] Dianion: An Intermolecular Effectâ^' Structural, Electronic and Magnetic Properties. European Journal of Inorganic Chemistry, 2003, 2003, 4187-4194.	2.0	10
168	In silico study of the interstellar prebiotic formation and delivery of glycine. Rendiconti Lincei, 2011, 22, 137-144.	2.2	10
169	Strained ring motif at silica surfaces: A quantum mechanical study of their reactivity towards protic molecules. Computational and Theoretical Chemistry, 2015, 1074, 168-177.	2.5	10
170	What is the structure of FeC5H6+?. Chemical Physics Letters, 1995, 240, 526-532.	2.6	9
171	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.	1.4	9
172	Coordination Properties of Lysine Interacting with Co(I) and Co(II). A Theoretical and Mass Spectrometry Study. Journal of Physical Chemistry A, 2008, 112, 12385-12392.	2.5	9
173	Coordination of (Glycyl)_nglycine (n= 1â^'3) to Co⁺and Co²⁺. Journal of Physical Chemistry A, 2009, 113, 8883-8892.	2.5	9
174	Mixed Adenine/Guanine Quartets with Three transâ€‹a₂Pt^{II} (a=NH₃ or MeNH₂) Crossâ€‹Links: Linkage and Rotational Isomerism, Base Pairing, and Loss of NH₃. Chemistry - A European Journal, 2014, 20, 3394-3407.	3.3	9
175	Computational study on donorâ€“acceptor optical markers for Alzheimer's disease: a game of charge transfer and electron delocalization. Physical Chemistry Chemical Physics, 2016, 18, 11634-11643.	2.8	9
176	Fluorous l-Carbidopa Precursors: Highly Enantioselective Synthesis and Computational Prediction of Bioactivity. Journal of Organic Chemistry, 2018, 83, 303-313.	3.2	9
177	Activating a Peroxo Ligand for Câ^'O Bond Formation. Angewandte Chemie - International Edition, 2019, 58, 3037-3041.	13.8	9
178	Aerobic intramolecular carbonâ€“hydrogen bond oxidation promoted by Cu(<scp>i</scp>) complexes. Dalton Transactions, 2020, 49, 14647-14655.	3.3	9
179	Atomistic fibrillar architectures of polar prion-inspired heptapeptides. Chemical Science, 2020, 11, 13143-13151.	7.4	9
180	Theoretical study of the 2A2î—¸2B2 separation of the alkali superoxides. Chemical Physics Letters, 1992, 197, 213-216.	2.6	8

#	Article	IF	Citations
181	Influence of ionization on the conformational preferences of peptide models. Ramachandran surfaces of Nâ€formylâ€glycine amide and Nâ€formylâ€alanine amide radical cations. Journal of Computational Chemistry, 2009, 30, 1771-1784.	3.3	8
182	Stability of transient Cu+AÎ² (1â€“16) species and influence of coordination and peptide configuration on superoxide formation. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	8
183	Surface morphology controls water dissociation on hydrated IrO₂ nanoparticles. Nanoscale, 2021, 13, 14480-14489.	5.6	8
184	Multiple Condensation Reactions Involving Pt^{II}/Pd^{II}â^'OH₂, Ptâ^'NH₃, and Cytosineâ^'NH₂ Groups: New Twists in Cisplatinâ^'Nucleobase Chemistry. Chemistry - A European Journal, 2016, 22, 13653-13668.	3.3	7
185	Impact of Cu(<scp>ii</scp>) and Al(<scp>iii</scp>) on the conformational landscape of amyloidÎ²₁₋₄₂. Physical Chemistry Chemical Physics, 2021, 23, 13023-13032.	2.8	7
186	Ab initio study of the reaction between Cl4Wî—»CH2 and ethylene. Computational and Theoretical Chemistry, 1991, 251, 37-47.	1.5	6
187	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.	3.1	6
188	Site-selective-induced isomerization of formamide. Physical Chemistry Chemical Physics, 2019, 21, 25626-25634.	2.8	6
189	Canonical Watsonâ€“Crick base pair interactions in Ï€â€‰â†'â€‰Ï€* type triplet states. Molecular Physics, 2006, 104, 925-931.	1.7	5
190	Nucleobase Stacking at Clay Edges, a Favorable Interaction for RNA/DNA Oligomerization. ACS Earth and Space Chemistry, 2019, 3, 1023-1033.	2.7	5
191	Unusual hydrogen bonds in [AH3â€“H3O]+ radical cations (A=C, Si, Ge, Sn and Pb). Chemical Physics Letters, 2004, 395, 27-32.	2.6	4
192	Theoretical study of ScCO2+. International Journal of Quantum Chemistry, 1997, 63, 523-528.	2.0	3
193	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.	2.9	2
194	The role of charge transfer in the photophysics of dithiophene-based (NIADs) fluorescent markers for amyloid-Î² detection. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	2
195	Fluorescent Markers for Amyloidâ€Î² Detection: Computational Insights. Israel Journal of Chemistry, 2017, 57, 686-698.	2.3	2
196	Intramolecular Photocycloaddition of 2(5H)-Furanones to Temporarily Tethered Terminal Alkenes as a Stereoselective Source of Enantiomerically Pure Polyfunctionalyzed Cyclobutanes. Journal of Organic Chemistry, 2018, 83, 3188-3199.	3.2	2
197	Activating a Peroxo Ligand for Câ^'O Bond Formation. Angewandte Chemie, 2019, 131, 3069-3073.	2.0	2
198	First-Principles Modeling of Protein/Surface Interactions. Polyglycine Secondary Structure Adsorption on the TiO₂ (101) Anatase Surface Adopting a Full Periodic Approach. Journal of Chemical Information and Modeling, 2021, 61, 5484-5498.	5.4	2

#	Article	IF	Citations
199	An ab initio study of the collinear reaction of Fe+ (4F) and Fe+ (6D) with H2. Journal of Chemical Physics, 1991, 94, 4352-4355.	3.0	1
200	Computational Simulations of Prebiotic Processes. Cellular Origin and Life in Extreme Habitats, 2012, , 345-362.	0.3	1
201	Effects of Ionization and Cationization on Intermolecular Proton Transfer Reactions in DNA base Pairs. , 2003, , 1231-1255.		1
202	Can Cu+-Exchanged Zeolites Store Molecular Hydrogen? An ab initio Periodic Study Compared with Low-Temperature FTIR.. ChemInform, 2004, 35, no.	0.0	0
203	Theoretical and computational chemistry in Spain. Theoretical Chemistry Accounts, 2011, 128, 389-391.	1.4	0
204	Computational simulations of copper complexes relevant to Alzheimer's disease. , 2014, , .		0
205	Insights on the binding of thioflavin derivative markers to amyloid fibril models and AÎ²1-40 fibrils from computational approaches. , 2014, , .		0
206	Frontispiece: When the Surface Matters: Prebiotic Peptide-Bond Formation on the TiO2 (101) Anatase Surface through Periodic DFT-D2 Simulations. Chemistry - A European Journal, 2018, 24, .	3.3	0
207	Frontispiece: Enhanced Metallophilicity in Metalâ€“Carbene Systems: Stronger Character of Aurophilic Interactions in Solution. Chemistry - A European Journal, 2020, 26, .	3.3	0
208	Atomistic insights into the structure of heptapeptide nanofibers. Journal of Chemical Physics, 2021, 155, 055101.	3.0	0
209	Formamide Dehydration and Condensation on Acidic Montmorillonite: Mechanistic Insights from Ab-Initio Periodic Simulations. Lecture Notes in Computer Science, 2020, , 502-512.	1.3	0