

Mariona Sodupe

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/7312642/publications.pdf>

Version: 2024-02-01

209
papers

8,290
citations

41258

49
h-index

64668

79
g-index

214
all docs

214
docs citations

214
times ranked

7124
citing authors

#	ARTICLE	IF	CITATIONS
1	Metal coordination determines the catalytic activity of IrO ₂ nanoparticles for the oxygen evolution reaction. <i>Journal of Catalysis</i> , 2022, 412, 78-86.	3.1	13
2	Importance of the oxyl character on the IrO ₂ surface dependent catalytic activity for the oxygen evolution reaction. <i>Journal of Catalysis</i> , 2021, 396, 192-201.	3.1	18
3	Atomistic insights into the structure of heptapeptide nanofibers. <i>Journal of Chemical Physics</i> , 2021, 155, 055101.	1.2	0
4	Surface morphology controls water dissociation on hydrated IrO ₂ nanoparticles. <i>Nanoscale</i> , 2021, 13, 14480-14489.	2.8	8
5	Impact of Cu(II) and Al(III) on the conformational landscape of amyloid ¹⁻⁴² . <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13023-13032.	1.3	7
6	pH-Responsive Self-Assembly of Amyloid Fibrils for Dual Hydrolase-Oxidase Reactions. <i>ACS Catalysis</i> , 2021, 11, 595-607.	5.5	49
7	First-Principles Modeling of Protein/Surface Interactions. Polyglycine Secondary Structure Adsorption on the TiO ₂ (101) Anatase Surface Adopting a Full Periodic Approach. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5484-5498.	2.5	2
8	BCN-M: A Free Computational Tool for Generating Wulff-like Nanoparticle Models with Controlled Stoichiometry. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1227-1237.	1.5	13
9	Enhanced Metallophilicity in Metal-Carbene Systems: Stronger Character of Auophilic Interactions in Solution. <i>Chemistry - A European Journal</i> , 2020, 26, 997-1002.	1.7	11
10	Aerobic intramolecular carbon-hydrogen bond oxidation promoted by Cu(I) complexes. <i>Dalton Transactions</i> , 2020, 49, 14647-14655.	1.6	9
11	Atomistic fibrillar architectures of polar prion-inspired heptapeptides. <i>Chemical Science</i> , 2020, 11, 13143-13151.	3.7	9
12	Frontispiece: Enhanced Metallophilicity in Metal-Carbene Systems: Stronger Character of Auophilic Interactions in Solution. <i>Chemistry - A European Journal</i> , 2020, 26, .	1.7	0
13	Formamide Dehydration and Condensation on Acidic Montmorillonite: Mechanistic Insights from Ab-Initio Periodic Simulations. <i>Lecture Notes in Computer Science</i> , 2020, , 502-512.	1.0	0
14	Role of Mineral Surfaces in Prebiotic Chemical Evolution. <i>In Silico Quantum Mechanical Studies</i> . <i>Life</i> , 2019, 9, 10.	1.1	44
15	Nucleobase Stacking at Clay Edges, a Favorable Interaction for RNA/DNA Oligomerization. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 1023-1033.	1.2	5
16	Water Adsorption on MO ₂ (M = Ti, Ru, and Ir) Surfaces. Importance of Octahedral Distortion and Cooperative Effects. <i>ACS Omega</i> , 2019, 4, 2989-2999.	1.6	28
17	Site-selective-induced isomerization of formamide. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 25626-25634.	1.3	6
18	Activating a Peroxo Ligand for C=O Bond Formation. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 3037-3041.	7.2	9

#	ARTICLE	IF	CITATIONS
19	Activating a Peroxo Ligand for C=O Bond Formation. <i>Angewandte Chemie</i> , 2019, 131, 3069-3073.	1.6	2
20	Interaction between Ruthenium Oxide Surfaces and Water Molecules. Effect of Surface Morphology and Water Coverage. <i>Journal of Physical Chemistry C</i> , 2019, 123, 7786-7798.	1.5	18
21	Intramolecular Photocycloaddition of 2(5 <i>H</i>)-Furanones to Temporarily Tethered Terminal Alkenes as a Stereoselective Source of Enantiomerically Pure Polyfunctionalized Cyclobutanes. <i>Journal of Organic Chemistry</i> , 2018, 83, 3188-3199.	1.7	2
22	Influence of Ligands and Oxidation State on the Reactivity of Pentacoordinated Iron Carbenes with Olefins: Metathesis versus Cyclopropanation. <i>Organometallics</i> , 2018, 37, 1229-1241.	1.1	14
23	How Does Silica Catalyze the Amide Bond Formation under Dry Conditions? Role of Specific Surface Silanol Pairs. <i>ACS Catalysis</i> , 2018, 8, 4558-4568.	5.5	51
24	Reactivity of Metal Carbenes with Olefins: Theoretical Insights on the Carbene Electronic Structure and Cyclopropanation Reaction Mechanism. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1702-1712.	1.1	26
25	Drastic Effect of the Peptide Sequence on the Copper Binding Properties of Tripeptides and the Electrochemical Behaviour of Their Copper(II) Complexes. <i>Chemistry - A European Journal</i> , 2018, 24, 5153-5162.	1.7	24
26	Fluorous I-Carbidopa Precursors: Highly Enantioselective Synthesis and Computational Prediction of Bioactivity. <i>Journal of Organic Chemistry</i> , 2018, 83, 303-313.	1.7	9
27	Frontispiece: When the Surface Matters: Prebiotic Peptide-Bond Formation on the TiO ₂ (101) Anatase Surface through Periodic DFT-D2 Simulations. <i>Chemistry - A European Journal</i> , 2018, 24, .	1.7	0
28	Formamide Adsorption at the Amorphous Silica Surface: A Combined Experimental and Computational Approach. <i>Life</i> , 2018, 8, 42.	1.1	14
29	Small molecule inhibits I \pm -synuclein aggregation, disrupts amyloid fibrils, and prevents degeneration of dopaminergic neurons. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 10481-10486.	3.3	166
30	When the Surface Matters: Prebiotic Peptide-Bond Formation on the TiO ₂ (101) Anatase Surface through Periodic DFT-D2 Simulations. <i>Chemistry - A European Journal</i> , 2018, 24, 16292-16301.	1.7	23
31	Enhanced photocatalytic activity of gold nanoparticles driven by supramolecular host-guest chemistry. <i>Chemical Communications</i> , 2017, 53, 2126-2129.	2.2	11
32	Elucidating the 3D structures of Al(III)-Al ²⁺ complexes: a template free strategy based on the pre-organization hypothesis. <i>Chemical Science</i> , 2017, 8, 5041-5049.	3.7	21
33	Visible-Light Photocatalytic Intramolecular Cyclopropane Ring Expansion. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 7826-7830.	7.2	47
34	Canonical, Deprotonated, or Zwitterionic? A Computational Study on Amino Acid Interaction with the TiO ₂ (101) Anatase Surface. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14156-14165.	1.5	28
35	Fluorescent Markers for Amyloid- β Detection: Computational Insights. <i>Israel Journal of Chemistry</i> , 2017, 57, 686-698.	1.0	2
36	Binding of Thioflavin T and Related Probes to Polymorphic Models of Amyloid- β Fibrils. <i>Journal of Physical Chemistry B</i> , 2017, 121, 8926-8934.	1.2	34

#	ARTICLE	IF	CITATIONS
37	The role of charge transfer in the photophysics of dithiophene-based (NIADs) fluorescent markers for amyloid- β^2 detection. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	2
38	Does Fe ²⁺ in olivine-based interstellar grains play any role in the formation of H ₂ ? Atomistic insights from DFT periodic simulations. <i>Chemical Communications</i> , 2016, 52, 6873-6876.	2.2	22
39	Toward Olefin Metathesis with Iron Carbene Complexes: Benefits of Tridentate σ -Donating Ligands. <i>Organometallics</i> , 2016, 35, 3914-3923.	1.1	32
40	Multiple Condensation Reactions Involving Pt ^{II} /Pd ^{II} -OH ₂ , Pt ^{II} -NH ₃ , and Cytosine ^{II} -NH ₂ Groups: New Twists in Cisplatin ^{II} -Nucleobase Chemistry. <i>Chemistry - A European Journal</i> , 2016, 22, 13653-13668.	1.7	7
41	Amide and Peptide Bond Formation: Interplay between Strained Ring Defects and Silanol Groups at Amorphous Silica Surfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24817-24826.	1.5	30
42	Computational study on donor-acceptor optical markers for Alzheimer's disease: a game of charge transfer and electron delocalization. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11634-11643.	1.3	9
43	Stability of transient Cu+Al ²⁺ (~ 16) species and influence of coordination and peptide configuration on superoxide formation. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	8
44	Strained ring motif at silica surfaces: A quantum mechanical study of their reactivity towards protic molecules. <i>Computational and Theoretical Chemistry</i> , 2015, 1074, 168-177.	1.1	10
45	Disaggregation-induced fluorescence enhancement of NIAD-4 for the optical imaging of amyloid- β^2 fibrils. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 19718-19725.	1.3	24
46	Modeling Cu ²⁺ -Al ²⁺ complexes from computational approaches. <i>AIP Advances</i> , 2015, 5, 092402.	0.6	17
47	Coordination properties of a metal chelator clioquinol to Zn ²⁺ studied by static DFT and ab initio molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 13582-13589.	1.3	13
48	Dioxygen activation in the Cu ^{II} -amyloid β^2 complex. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 27270-27274.	1.3	24
49	Relevance of silicate surface morphology in interstellar H ₂ formation. Insights from quantum chemical calculations. <i>Monthly Notices of the Royal Astronomical Society</i> , 2015, 453, 914-924.	1.6	23
50	Thioflavin-based molecular probes for application in Alzheimer's disease: from in silico to in vitro models. <i>Metallomics</i> , 2015, 7, 83-92.	1.0	23
51	Computational simulations of copper complexes relevant to Alzheimer's disease. , 2014, , .		0
52	Insights on the binding of thioflavin derivative markers to amyloid fibril models and Al ²⁺ 1-40 fibrils from computational approaches. , 2014, , .		0
53	3-Hydroxy-4-pyridinone derivatives as metal ion and amyloid binding agents. <i>Metallomics</i> , 2014, 6, 249-262.	1.0	19
54	DFT Study on the Relative Stabilities of Substituted Ruthenacyclobutane Intermediates Involved in Olefin Cross-Metathesis Reactions and Their Interconversion Pathways. <i>Organometallics</i> , 2014, 33, 6065-6075.	1.1	31

#	ARTICLE	IF	CITATIONS
55	Interstellar H adsorption and H ₂ formation on the crystalline (010) forsterite surface: a B3LYP-D2* periodic study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17447-17457.	1.3	28
56	3D Structures and Redox Potentials of Cu ²⁺ –Al ²⁺ (16) Complexes at Different pH: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4840-4850.	1.2	30
57	B3LYP Periodic Study of the Physicochemical Properties of the Nonpolar (010) Mg-Pure and Fe-Containing Olivine Surfaces. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5866-5875.	1.1	20
58	Gas-Phase and Microsolvated Glycine Interacting with Boron Nitride Nanotubes. A B3LYP-D2* Periodic Study. <i>Inorganics</i> , 2014, 2, 334-350.	1.2	15
59	Mixed Adenine/Guanine Quartets with Three <i>trans</i> -Pt ^{II} (a=NH ₃ or MeNH ₂) Crosslinks: Linkage and Rotational Isomerism, Base Pairing, and Loss of NH ₃ . <i>Chemistry - A European Journal</i> , 2014, 20, 3394-3407.	1.7	9
60	Physisorption vs. chemisorption of probe molecules on boron nitride nanomaterials: the effect of surface curvature. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13190.	1.3	30
61	Structural Behaviors of Cytosine into the Hydrated Interlayer of Na ⁺ -Montmorillonite Clay. An ab Initio Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 26179-26189.	1.5	17
62	<i>Exo/endo</i> Selectivity of the Ring-Closing Enyne Methathesis Catalyzed by Second Generation Ru-Based Catalysts. Influence of Reactant Substituents. <i>ACS Catalysis</i> , 2013, 3, 206-218.	5.5	31
63	Silica Surface Features and Their Role in the Adsorption of Biomolecules: Computational Modeling and Experiments. <i>Chemical Reviews</i> , 2013, 113, 4216-4313.	23.0	508
64	Thioflavin-T excimer formation upon interaction with amyloid fibers. <i>Chemical Communications</i> , 2013, 49, 5745.	2.2	56
65	Insights on the Binding of Thioflavin Derivative Markers to Amyloid-Like Fibril Models from Quantum Chemical Calculations. <i>Journal of Physical Chemistry B</i> , 2013, 117, 6674-6680.	1.2	19
66	Surface Reaction of Acetylene with H-Terminated Silicon Surfaces. A Theoretical Study from Hybrid DFT-D2 Periodic Simulations. <i>Journal of Physical Chemistry C</i> , 2013, 117, 15130-15138.	1.5	6
67	DFT Study on the Recovery of Hoveyda–Grubbs Type Catalyst Precursors in Enyne and Diene Ring-Closing Metathesis. <i>Chemistry - A European Journal</i> , 2013, 19, 14553-14565.	1.7	30
68	COMPUTATIONAL STUDY OF INTERSTELLAR GLYCINE FORMATION OCCURRING AT RADICAL SURFACES OF WATER-ICE DUST PARTICLES. <i>Astrophysical Journal</i> , 2012, 754, 24.	1.6	51
69	On the electronic structure of second generation Hoveyda–Grubbs alkene metathesis precursors. <i>Computational and Theoretical Chemistry</i> , 2012, 996, 57-67.	1.1	21
70	Differences in the Activation Processes of Phosphine-Containing and Grubbs–Hoveyda-Type Alkene Metathesis Catalysts. <i>Organometallics</i> , 2012, 31, 4203-4215.	1.1	85
71	Theoretical study of the adsorption of DNA bases on the acidic external surface of montmorillonite. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 945-954.	1.3	39
72	Cooperative effects at water–crystalline silica interfaces strengthen surface silanol hydrogen bonding. An ab initio molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10507.	1.3	43

#	ARTICLE	IF	CITATIONS
73	Computational Simulations of Prebiotic Processes. Cellular Origin and Life in Extreme Habitats, 2012, , 345-362.	0.3	1
74	Prebiotic chemistry. Chemical Society Reviews, 2012, 41, 5373.	18.7	13
75	Oâ€“O Bond activation in H ₂ O ₂ and (CH ₃) ₃ C-OOH mediated by [Ni(cyclam)(CH ₃ CN) ₂](ClO ₄) ₂ : Different mechanisms to form the same Ni(III) product?. Dalton Transactions, 2011, 40, 6868.	1.6	15
76	Three Dimensional Models of Cu ²⁺ -Al ²⁺ (1â€“16) Complexes from Computational Approaches. Journal of the American Chemical Society, 2011, 133, 15008-15014.	6.6	61
77	Computational calculations of pKa values of imidazole in Cu(II) complexes of biological relevance. Physical Chemistry Chemical Physics, 2011, 13, 7852.	1.3	55
78	Ab Initio Design of Chelating Ligands Relevant to Alzheimerâ€™s Disease: Influence of Metalloaromaticity. Journal of Physical Chemistry A, 2011, 115, 12659-12666.	1.1	20
79	Do H-Bond Features of Silica Surfaces Affect the H ₂ O and NH ₃ Adsorption? Insights from Periodic B3LYP Calculations. Journal of Physical Chemistry A, 2011, 115, 11221-11228.	1.1	25
80	Structures and Stabilities of Fe ^{2+/3+} Complexes Relevant to Alzheimerâ€™s Disease: An ab Initio Study. Journal of Physical Chemistry A, 2011, 115, 12523-12530.	1.1	27
81	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.	1.3	14
82	On the mechanism of the N-glycosidic bond hydrolysis of 2â€“deoxyguanosine: insights from first principles calculations. Theoretical Chemistry Accounts, 2011, 128, 619-626.	0.5	14
83	Theoretical and computational chemistry in Spain. Theoretical Chemistry Accounts, 2011, 128, 389-391.	0.5	0
84	In silico study of the interstellar prebiotic formation and delivery of glycine. Rendiconti Lincei, 2011, 22, 137-144.	1.0	10
85	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.	1.7	56
86	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.	1.7	14
87	DFT Mechanistic Study on Diene Metathesis Catalyzed by Ruâ€“Based Grubbsâ€™ Hoveydaâ€“Type Carbenes: The Key Role of Î€Electron Density Delocalization in the Hoveyda Ligand. Chemistry - A European Journal, 2010, 16, 7331-7343.	1.7	78
88	Crystal structure of thioflavin-T and its binding to amyloid fibrils: insights at the molecular level. Chemical Communications, 2010, 46, 1156.	2.2	78
89	The Role of Exact Exchange in the Description of Cu ²⁺ -â€“(H ₂ O) _n (n = 1â€“6) Complexes by Means of DFT Methods. Journal of Physical Chemistry A, 2010, 114, 10857-10863.	1.1	43
90	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.	1.5	20

#	ARTICLE	IF	CITATIONS
91	[2 + 2] Photocycloaddition of 2(5 <i>H</i>)-Furanone to Unsaturated Compounds. Insights from First Principles Calculations and Transient-Absorption Measurements. <i>Journal of Organic Chemistry</i> , 2010, 75, 4392-4401.	1.7	17
92	Ab initio molecular dynamics study of the hydration of Li ⁺ , Na ⁺ and K ⁺ in a montmorillonite model. Influence of isomorphic substitution. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 688-697.	1.3	90
93	Periodic DFT Study of Radical Species on Crystalline Silica Surfaces. <i>Journal of Physical Chemistry C</i> , 2010, 114, 16430-16438.	1.5	27
94	A DFT periodic study on the interaction between O ₂ and cation exchanged chabazite MCHA (M = H ⁺ , Na ⁺ or Cu ⁺): effects in the triplet-singlet energy gap. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 442-452.	1.3	19
95	Deep-space glycine formation via Strecker-type reactions activated by ice water dust mantles. A computational approach. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5285.	1.3	77
96	Formation versus Hydrolysis of the Peptide Bond from a Quantum-mechanical Viewpoint: The Role of Mineral Surfaces and Implications for the Origin of Life. <i>International Journal of Molecular Sciences</i> , 2009, 10, 746-760.	1.8	24
97	Influence of ionization on the conformational preferences of peptide models. Ramachandran surfaces of <i>N</i> -formylglycine amide and <i>N</i> -formylalanine amide radical cations. <i>Journal of Computational Chemistry</i> , 2009, 30, 1771-1784.	1.5	8
98	Influence of π -stacking on the N7 and O6 proton affinity of guanine. <i>Theoretical Chemistry Accounts</i> , 2009, 123, 105-111.	0.5	11
99	Structure, Bonding, and Relative Stability of the Ground and Low-Lying Electronic States of CuO ₂ . The Role of Exact Exchange. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1308-1317.	1.1	19
100	Theoretical Study of the Adsorption of RNA/DNA Bases on the External Surfaces of Na ⁺ -Montmorillonite. <i>Journal of Physical Chemistry C</i> , 2009, 113, 13741-13749.	1.5	72
101	Coordination of (Glycyl)glycine (<i>n</i> = 1-3) to Co ²⁺ and Co ³⁺ . <i>Journal of Physical Chemistry A</i> , 2009, 113, 8883-8892.	1.1	9
102	H-Bond Features of Fully Hydroxylated Surfaces of Crystalline Silica Polymorphs: A Periodic B3LYP Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 17876-17884.	1.5	54
103	Affinity Scale for the Interaction of Amino Acids with Silica Surfaces. <i>Journal of Physical Chemistry C</i> , 2009, 113, 5741-5750.	1.5	105
104	Design, Selection, and Characterization of Thioflavin-Based Intercalation Compounds with Metal Chelating Properties for Application in Alzheimer's Disease. <i>Journal of the American Chemical Society</i> , 2009, 131, 1436-1451.	6.6	196
105	Realistic Models of Hydroxylated Amorphous Silica Surfaces and MCM-41 Mesoporous Material Simulated by Large-scale Periodic B3LYP Calculations. <i>Advanced Materials</i> , 2008, 20, 4579-4583.	11.1	199
106	How the site of ionisation influences side-chain fragmentation in histidine radical cation. <i>Chemical Physics Letters</i> , 2008, 451, 276-281.	1.2	14
107	Cu ²⁺ Cation Coordination to Adenine-Thymine Base Pair. Effects on Intermolecular Proton-Transfer Processes. <i>Journal of Physical Chemistry B</i> , 2008, 112, 4817-4825.	1.2	52
108	Binding Properties of Cu ²⁺ -(glycyl)glycine Complexes (<i>n</i> = 1, 2)	1.1	19

#	ARTICLE	IF	CITATIONS
109	Coordination Properties of Lysine Interacting with Co(I) and Co(II). A Theoretical and Mass Spectrometry Study. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12385-12392.	1.1	9
110	Influence of the Side Chain in the Structure and Fragmentation of Amino Acids Radical Cations. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2210-2220.	2.3	41
111	On the Bonding of First-Row Transition Metal Cations to Guanine and Adenine Nucleobases. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9823-9829.	1.1	34
112	Aluminosilicate Surfaces as Promoters for Peptide Bond Formation: An Assessment of Bernal's Hypothesis by ab Initio Methods. <i>Journal of the American Chemical Society</i> , 2007, 129, 8333-8344.	6.6	75
113	Influence of N7 Protonation on the Mechanism of the N-Glycosidic Bond Hydrolysis in 2'-Deoxyguanosine. A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2007, 111, 6071-6077.	1.2	42
114	Is the Peptide Bond Formation Activated by Cu ²⁺ Interactions? Insights from Density Functional Calculations. <i>Journal of Physical Chemistry B</i> , 2007, 111, 5740-5747.	1.2	32
115	Effects of protonation on proton transfer processes in Watson-Crick adenine-thymine base pair. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 113-121.	0.5	36
116	Gas-phase proton-transport self-catalysed isomerisation of glutamine radical cation: The important role of the side-chain. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 589-595.	0.5	9
117	Interaction of Glycine with Isolated Hydroxyl Groups at the Silica Surface: First Principles B3LYP Periodic Simulation. <i>Langmuir</i> , 2006, 22, 6593-6604.	1.6	83
118	Canonical Watson-Crick base pair interactions in π - π^* type triplet states. <i>Molecular Physics</i> , 2006, 104, 925-931.	0.8	5
119	Cation- π Interactions and Oxidative Effects on Cu ⁺ and Cu ²⁺ Binding to Phe, Tyr, Trp, and His Amino Acids in the Gas Phase. Insights from First-Principles Calculations. <i>Journal of Physical Chemistry B</i> , 2006, 110, 24189-24199.	1.2	77
120	Palladium Nanoparticles Entrapped in Heavily Fluorinated Compounds. <i>Chemistry of Materials</i> , 2006, 18, 716-722.	3.2	38
121	Effects of Ionization, Metal Cationization and Protonation on 2'-Deoxyguanosine: Changes on Sugar Puckering and Stability of the N-Glycosidic Bond. <i>Journal of Physical Chemistry B</i> , 2006, 110, 5767-5772.	1.2	24
122	Gas phase reactivity of Cu ⁺ -aromatic amino acids. <i>International Journal of Mass Spectrometry</i> , 2006, 257, 60-69.	0.7	24
123	A Theoretical Study on PdII Complexes Containing Hemilabile Pyrazole-Derived Ligands. <i>European Journal of Inorganic Chemistry</i> , 2006, 2006, 447-454.	1.0	18
124	Does Silica Surface Catalyse Peptide Bond Formation? New Insights from First-Principles Calculations. <i>ChemPhysChem</i> , 2006, 7, 157-163.	1.0	77
125	Effects of ionization on N-glycylglycine peptide: Influence of intramolecular hydrogen bonds. <i>Journal of Chemical Physics</i> , 2006, 124, 154306.	1.2	26
126	Structure and fragmentation of glycine, alanine, serine and cysteine radical cations. A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2005, 727, 191-197.	1.5	63

#	ARTICLE	IF	CITATIONS
127	Peptide bond formation activated by the interplay of Lewis and Brønsted catalysts. <i>Chemical Physics Letters</i> , 2005, 408, 295-301.	1.2	35
128	Coordination properties of glycylglycine to Cu ⁺ , Ni ⁺ and Co ⁺ . Influence of metal cation electronic configuration. <i>New Journal of Chemistry</i> , 2005, 29, 1585.	1.4	32
129	Hydrogen Bond vs Proton Transfer in HZSM5 Zeolite. A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 19301-19308.	1.2	22
130	Hydrogen bonding and aromaticity in the guanine-cytosine base pair interacting with metal cations (M ⁺ =Cu ⁺ , Ca ²⁺ and Cu ²⁺). <i>Molecular Physics</i> , 2005, 103, 163-173.	0.8	32
131	Coordination Properties of the Oxime Analogue of Glycine to Cu(II). <i>Journal of Physical Chemistry A</i> , 2005, 109, 5668-5676.	1.1	46
132	Adsorption of NH ₃ and H ₂ O in Acidic Chabazite. Comparison of ONIOM Approach with Periodic Calculations. <i>Journal of Physical Chemistry B</i> , 2005, 109, 3539-3545.	1.2	96
133	Interaction of Co ⁺ and Co ²⁺ with Glycine. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 224-230.	1.1	42
134	Water-catalyzed isomerization of the glycine radical cation. From hydrogen-atom transfer to proton-transport catalysis. <i>Theoretical Chemistry Accounts</i> , 2004, 111, 217-222.	0.5	26
135	Effects of protonation on proton-transfer processes in guanine-cytosine Watson-Crick base pairs. <i>Theoretical Chemistry Accounts</i> , 2004, 112, 318.	0.5	48
136	Metal-Mediated Deamination of Cytosine: Experiment and DFT Calculations. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 5396-5399.	7.2	33
137	Can Cu ⁺ -Exchanged Zeolites Store Molecular Hydrogen? An ab initio Periodic Study Compared with Low-Temperature FTIR. <i>ChemInform</i> , 2004, 35, no.	0.1	0
138	Unusual hydrogen bonds in [AH ₃ -H ₃ O] ⁺ radical cations (A=C, Si, Ge, Sn and Pb). <i>Chemical Physics Letters</i> , 2004, 395, 27-32.	1.2	4
139	Triplet (Ī, Ī*) Reactivity of the Guanine-Cytosine DNA Base Pair: Benign Deactivation versus Double Tautomerization via Intermolecular Hydrogen Transfer. <i>Journal of the American Chemical Society</i> , 2004, 126, 12770-12771.	6.6	23
140	Can Cu ⁺ -Exchanged Zeolites Store Molecular Hydrogen? An Ab-Initio Periodic Study Compared with Low-Temperature FTIR. <i>Journal of Physical Chemistry B</i> , 2004, 108, 8278-8286.	1.2	91
141	A Quantum Chemical Study of Cu ²⁺ Interacting with Guanine-Cytosine Base Pair. Electrostatic and Oxidative Effects on Intermolecular Proton-Transfer Processes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 333-341.	1.1	106
142	Electron hole formation in acidic zeolite catalysts. <i>Journal of Chemical Physics</i> , 2004, 121, 6034-6041.	1.2	49
143	Ground and Low-Lying States of Cu ²⁺ -H ₂ O. A Difficult Case for Density Functional Methods. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6072-6078.	1.1	85
144	Unusual hydrogen bonds in [AH ₃ -H ₃ O] ⁺ radical cations (A=C, Si, Ge, Sn and Pb) Single-electron hydrogen bond, proton-hydride hydrogen bond and formation of [H ₂ AOH ₂] ⁺ -H ₂ complexes. <i>Chemical Physics Letters</i> , 2004, 395, 27-32.	1.2	12

#	ARTICLE	IF	CITATIONS
145	Bent and Linear Forms of the (1/4-Oxo)bis[trichloroferrate(III)] Dianion: An Intermolecular Effect [†] Structural, Electronic and Magnetic Properties. <i>European Journal of Inorganic Chemistry</i> , 2003, 2003, 4187-4194.	1.0	10
146	Basic and acidic bifunctional catalysis: application to the tautomeric equilibrium of formamide. <i>Chemical Physics</i> , 2003, 295, 151-158.	0.9	12
147	Spin-forbidden N ₂ O dissociation in Cu ⁺ /ZSM-5. <i>Chemical Physics Letters</i> , 2003, 368, 242-246.	1.2	30
148	Gas Phase Dissociation Energies of Saturated AHn ⁺ Radical Cations and AHn Neutrals (A = Li ⁺ , F, Na ⁺ , Cl): [†] Dehydrogenation, Deprotonation, and Formation of AHn-2 ⁺ H ₂ Complexes. <i>Journal of the American Chemical Society</i> , 2003, 125, 7461-7469.	6.6	18
149	Gas Phase Reactivity of Ni ⁺ with Urea. <i>Mass Spectrometry and Theoretical Studies. Journal of Physical Chemistry A</i> , 2003, 107, 9865-9874.	1.1	18
150	Effects of Ionization and Cationization on Intermolecular Proton Transfer Reactions in DNA base Pairs. , 2003, , 1231-1255.		1
151	Isomerization versus Fragmentation of Glycine Radical Cation in Gas Phase. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5697-5702.	1.1	49
152	Keto [→] Enol Isomerization of Acetaldehyde in HZSM5. A Theoretical Study Using the ONIOM2 Method. <i>Journal of Physical Chemistry B</i> , 2002, 106, 10220-10226.	1.2	46
153	On the NO Decomposition by Cu ⁺ /ZSM-5 through the ZCu(NO ₂)(NO) or ZCu(N ₂ O ₃) Intermediates. <i>Journal of Physical Chemistry B</i> , 2002, 106, 1372-1379.	1.2	25
154	Effect of Counterpoise Correction on the Geometries and Vibrational Frequencies of Hydrogen Bonded Systems. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4359-4364.	1.1	57
155	Gas-Phase Reactivity of Ni ⁺ with Glycine. <i>Journal of Physical Chemistry A</i> , 2001, 105, 5340-5347.	1.1	66
156	Solvent-assisted catalysis in the enolization of acetaldehyde radical cation. <i>Chemical Physics Letters</i> , 2001, 334, 112-118.	1.2	52
157	Protonation of glycine, serine and cysteine. Conformations, proton affinities and intrinsic basicities. <i>Computational and Theoretical Chemistry</i> , 2001, 537, 307-318.	1.5	83
158	Gas Phase Intramolecular Proton Transfer in Cationized Glycine and Chlorine Substituted Derivatives (M ⁺ =Gly, M=Na ⁺ , Mg ²⁺ , Cu ⁺ , Ni ⁺ , and Cu ²⁺): Existence of Zwitterionic Structures?. <i>Chemistry - A European Journal</i> , 2000, 6, 4393-4399.	1.7	60
159	Theoretical Study of the Structure of ZCu(NO ₂)(NO). A Proposed Intermediate in the NO _x Decomposition by Cu ⁺ /ZSM-5. <i>Journal of Physical Chemistry A</i> , 2000, 104, 3225-3230.	1.1	25
160	Intramolecular Proton Transfer in Glycine Radical Cation. <i>Journal of Physical Chemistry A</i> , 2000, 104, 1256-1261.	1.1	59
161	The Different Nature of Bonding in Cu ⁺ -Glycine and Cu ²⁺ -Glycine. <i>Journal of Physical Chemistry B</i> , 1999, 103, 2310-2317.	1.2	198
162	Density functional cluster model study of bonding and coordination modes of CO ₂ on Pd(111). <i>Surface Science</i> , 1999, 431, 208-219.	0.8	21

#	ARTICLE	IF	CITATIONS
163	Ground State of the (H ₂ O) ₂ ⁺ Radical Cation: A DFT versus Post-Hartree-Fock Methods. Journal of Physical Chemistry A, 1999, 103, 166-170.	1.1	232
164	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.	6.6	48
165	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.	6.6	203
166	Coordination of NO ₂ to Alkaline-Earth Metals. A Theoretical Study. Journal of Physical Chemistry A, 1998, 102, 630-635.	1.1	10
167	Coordination of NO ₂ to Cu and Mg in M(NO ₂) ₂ Complexes. A Theoretical Study. Inorganic Chemistry, 1998, 37, 4512-4517.	1.9	11
168	Coordination of Cu ⁺ Ions to Zeolite Frameworks Strongly Enhances Their Ability To Bind NO ₂ . An ab Initio Density Functional Study. Journal of the American Chemical Society, 1998, 120, 1545-1551.	6.6	109
169	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.	6.6	55
170	Theoretical Study of the Ionization of Phenol-Water and Phenol-Ammonia Hydrogen-Bonded Complexes. Journal of Physical Chemistry A, 1997, 101, 9142-9151.	1.1	76
171	Theoretical Study of M ⁺ CO ₂ and OM+CO Systems for First Transition Row Metal Atoms. Journal of Physical Chemistry A, 1997, 101, 7854-7859.	1.1	112
172	Theoretical study of ScCO ₂ ⁺ . International Journal of Quantum Chemistry, 1997, 63, 523-528.	1.0	3
173	Atomic reference energies for density functional calculations. Chemical Physics Letters, 1997, 265, 481-489.	1.2	154
174	Theoretical study of the ScCO ₂ + OScCO reaction. Computational and Theoretical Chemistry, 1996, 371, 79-84.	1.5	15
175	Comparison of density functional and coupled cluster methods in the study of metal-ligand systems: Sc-CO ₂ and Cu-NO ₂ . Journal of Chemical Physics, 1996, 105, 9966-9971.	1.2	46
176	What is the structure of FeC ₅ H ₆ ⁺ ?. Chemical Physics Letters, 1995, 240, 526-532.	1.2	9
177	Theoretical study of the bonding of NO ₂ to Cu and Ag. Journal of Chemical Physics, 1995, 103, 9738-9743.	1.2	21
178	Theoretical Study of the Ionization of the H ₂ S-H ₂ S, PH ₃ -H ₂ S, and ClH-H ₂ S Hydrogen Bonded Molecules. Journal of the American Chemical Society, 1995, 117, 8416-8421.	6.6	28
179	On the Bonding in Sc-CO ₂ . The Journal of Physical Chemistry, 1995, 99, 8567-8571.	2.9	41
180	A study of the ground and low-lying states of MgC ₂ H ₂ ⁺ and MgC ₂ H ₄ ⁺ . Chemical Physics, 1994, 185, 163-171.	0.9	25

#	ARTICLE	IF	CITATIONS
181	Theoretical Study of the Ionization of the H ₂ O-H ₂ O, NH ₃ -H ₂ O, and FH-H ₂ O Hydrogen-Bonded Molecules. <i>Journal of the American Chemical Society</i> , 1994, 116, 8249-8258.	6.6	51
182	The bonding in FeC ₅ H ⁺ . <i>Chemical Physics Letters</i> , 1993, 207, 19-22.	1.2	14
183	The bonding in the low-lying states of MgO ⁺ . <i>Chemical Physics Letters</i> , 1993, 203, 215-219.	1.2	16
184	A theoretical study of the spectroscopy of SrH ₂ O ⁺ and SrNH ₃ ⁺ . <i>Chemical Physics Letters</i> , 1993, 212, 624-630.	1.2	11
185	A study of the ground and low-lying states of MgCH ⁺ . <i>Chemical Physics Letters</i> , 1993, 214, 489-494.	1.2	28
186	Determination of the structure and bond energies of nickel dioxide and copper dioxide. <i>The Journal of Physical Chemistry</i> , 1993, 97, 856-859.	2.9	53
187	Comment on: Anabinitio study of the ionization of sodium superoxide. <i>Journal of Chemical Physics</i> , 1992, 96, 7871-7871.	1.2	11
188	Theoretical study of the bonding of the first-row transition-metal positive ions to ethylene. [Erratum to document cited in CA116(13):128993g]. <i>The Journal of Physical Chemistry</i> , 1992, 96, 5670-5670.	2.9	2
189	Theoretical study of the alkaline-earth metal superoxides BeO ₂ through SrO ₂ . <i>The Journal of Physical Chemistry</i> , 1992, 96, 9259-9264.	2.9	35
190	Theoretical study of the bonding of the first-row transition-metal positive ions to ethylene. <i>The Journal of Physical Chemistry</i> , 1992, 96, 2118-2122.	2.9	101
191	A theoretical study of the positive and dipositive ions of M(NH ₃) _n and M(H ₂ O) _n for M=Mg, Ca, or Sr. <i>Journal of Chemical Physics</i> , 1992, 96, 4453-4463.	1.2	206
192	Gas-phase chemistry of Sc(CH ₃) ₂ ⁺ with alkenes: activation of allylic carbon-hydrogen (C-H) bonds by a d ₀ system and the migratory insertion of C:C bonds into scandium-methyl (Sc ⁺ -CH ₃) bonds. <i>Journal of the American Chemical Society</i> , 1992, 114, 9106-9111.	6.6	15
193	The calculation of the vibrational frequencies of CuCO ⁺ , NiCO and CuCH ₃ . <i>Chemical Physics Letters</i> , 1992, 189, 266-272.	1.2	49
194	A theoretical study of the spectroscopy of MgH ₂ O ⁺ and MgCH ₃ OH ⁺ . <i>Chemical Physics Letters</i> , 1992, 195, 494-499.	1.2	50
195	A theoretical study of Mg(CO ₂) _n and Sr(CO ₂) _n for n = 1 and 2 and Mg ₂ CO ₂ . <i>Chemical Physics Letters</i> , 1992, 192, 185-194.	1.2	59
196	Theoretical study of the 2A ₂ ⁻ –2B ₂ separation of the alkali superoxides. <i>Chemical Physics Letters</i> , 1992, 197, 213-216.	1.2	8
197	Theoretical determination of the alkali-metal superoxide bond energies. <i>Chemical Physics Letters</i> , 1992, 195, 200-206.	1.2	48
198	Chemistry of the scandium-benzyne ion in the gas phase. <i>Inorganic Chemistry</i> , 1991, 30, 3822-3829.	1.9	22

#	ARTICLE	IF	CITATIONS
199	Diels-Alder cycloadditions of electron-rich, electron-deficient, and push-pull dienes with cyclic dienophiles: high-pressure-induced reactions and theoretical calculations. <i>Journal of Organic Chemistry</i> , 1991, 56, 4135-4141.	1.7	37
200	An ab initio study of the collinear reaction of Fe+ (4F) and Fe+ (6D) with H ₂ . <i>Journal of Chemical Physics</i> , 1991, 94, 4352-4355.	1.2	1
201	Theoretical study of the bonding of the first- and second-row transition-metal positive ions to acetylene. <i>The Journal of Physical Chemistry</i> , 1991, 95, 8640-8645.	2.9	100
202	Theoretical study of one and two ammonia molecules bound to the first-row transition metal ions. <i>The Journal of Physical Chemistry</i> , 1991, 95, 10677-10681.	2.9	90
203	Ab initio study of the reaction between Cl ₄ W ⁺ →CH ₂ and ethylene. <i>Computational and Theoretical Chemistry</i> , 1991, 251, 37-47.	1.5	6
204	Al ⁺ ligand binding energies. <i>Chemical Physics Letters</i> , 1991, 181, 321-326.	1.2	42
205	The metal ligand binding energies for Sr(H ₂ O) _n . <i>Journal of Chemical Physics</i> , 1991, 95, 9422-9423.	1.2	11
206	Ab initio study of the ground and low-lying states of FeH. <i>Journal of Chemical Physics</i> , 1990, 92, 2478-2480.	1.2	24
207	Ground and low-lying states of FeH ⁺ as derived from ab initio self-consistent field and configuration interaction calculations. <i>Journal of Chemical Physics</i> , 1989, 90, 6436-6442.	1.2	19
208	Theoretical study of the conformational preferences in the Cl ₄ W:CH ₂ complex. <i>Organometallics</i> , 1989, 8, 1837-1841.	1.1	16
209	An AM1 and MNDO theoretical study of the Diels-Alder reaction between .beta.-angelica lactone and cyclopentadiene. <i>Journal of Organic Chemistry</i> , 1989, 54, 2488-2490.	1.7	17