Albert Rimola

List of Publications by Year
in descending order

122 papers	4,215 citations	101384 36 h-index	133063 59 g-index
129 all docs	129 docs citations	129 times ranked	4154 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.	23.0	508
2	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.	6.6	196
3	Hydroxyapatite as a key biomaterial: quantum-mechanical simulation of its surfaces in interaction with biomolecules. Physical Chemistry Chemical Physics, 2010, 12, 6309.	1.3	136
4	Seeds Of Life In Space (SOLIS): The Organic Composition Diversity at 300â€“1000 au Scale in Solar-type Star-forming Regions[*]. Astrophysical Journal, 2017, 850, 176.	1.6	116
5	Affinity Scale for the Interaction of Amino Acids with Silica Surfaces. Journal of Physical Chemistry C, 2009, 113, 5741-5750.	1.5	105
6	Seeds of Life in Space (SOLIS). Astronomy and Astrophysics, 2017, 605, L3.	2.1	98
7	Ab Initio Modeling of Protein/Biomaterial Interactions: Glycine Adsorption at Hydroxyapatite Surfaces. Journal of the American Chemical Society, 2008, 130, 16181-16183.	6.6	97
8	Combined quantum chemical and modeling study of CO hydrogenation on water ice. Astronomy and Astrophysics, 2014, 572, A70.	2.1	87
9	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.	1.1	85
10	Interaction of Glycine with Isolated Hydroxyl Groups at the Silica Surface:â€‰ First Principles B3LYP Periodic Simulation. Langmuir, 2006, 22, 6593-6604.	1.6	83
11	Can Formamide Be Formed on Interstellar Ice? An Atomistic Perspective. ACS Earth and Space Chemistry, 2018, 2, 720-734.	1.2	83
12	Crystal structure of thioflavin-T and its binding to amyloid fibrils: insights at the molecular level. Chemical Communications, 2010, 46, 1156.	2.2	78
13	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.	1.2	77
14	Does Silica Surface Catalyse Peptide Bond Formation? New Insights from First-Principles Calculations. ChemPhysChem, 2006, 7, 157-163.	1.0	77
15	Deep-space glycine formation via Strecker-type reactions activated by ice water dust mantles. A computational approach. Physical Chemistry Chemical Physics, 2010, 12, 5285.	1.3	77
16	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.	6.6	75
17	Binding Energies of Interstellar Molecules on Crystalline and Amorphous Models of Water Ice by Ab Initio Calculations. Astrophysical Journal, 2020, 904, 11.	1.6	65
18	Physisorption of aromatic organic contaminants at the surface of hydrophobic/hydrophilic silica geosorbents: a B3LYP-D modeling study. Physical Chemistry Chemical Physics, 2010, 12, 6357.	1.3	60

#	Article	IF	Citations
19	The (impossible?) formation of acetaldehyde on the grain surfaces: insights from quantum chemical calculations. Monthly Notices of the Royal Astronomical Society: Letters, 2016, 459, L6-L10.	1.2	56
20	Reactivity of HCO with CH₃ and NH₂ on Water Ice Surfaces. A Comprehensive Accurate Quantum Chemistry Study. ACS Earth and Space Chemistry, 2019, 3, 2158-2170.	1.2	55
21	Thermal Desorption of Interstellar Ices: A Review on the Controlling Parameters and Their Implications from Snowlines to Chemical Complexity. ACS Earth and Space Chemistry, 2022, 6, 597-630.	1.2	55
22	Seeds of Life in Space (SOLIS). Astronomy and Astrophysics, 2017, 605, A57.	2.1	54
23	The mechanism of hexamethylenetetramine (HMT) formation in the solid state at low temperature. Physical Chemistry Chemical Physics, 2012, 14, 12309.	1.3	52
24	COMPUTATIONAL STUDY OF INTERSTELLAR GLYCINE FORMATION OCCURRING AT RADICAL SURFACES OF WATER-ICE DUST PARTICLES. Astrophysical Journal, 2012, 754, 24.	1.6	51
25	Does Adsorption at Hydroxyapatite Surfaces Induce Peptide Folding? Insights from Large-Scale B3LYP Calculations. Journal of the American Chemical Society, 2012, 134, 10899-10910.	6.6	51
26	How Does Silica Catalyze the Amide Bond Formation under Dry Conditions? Role of Specific Surface Silanol Pairs. ACS Catalysis, 2018, 8, 4558-4568.	5.5	51
27	Neutral vs Zwitterionic Glycine Forms at the Water/Silica Interface: Structure, Energies, and Vibrational Features from B3LYP Periodic Simulations. Langmuir, 2008, 24, 14027-14034.	1.6	47
28	A quantum mechanical study of the reactivity of (SiO)2-defective silica surfaces. Journal of Chemical Physics, 2008, 128, 204702.	1.2	45
29	Role of Mineral Surfaces in Prebiotic Chemical Evolution. In Silico Quantum Mechanical Studies. Life, 2019, 9, 10.	1.1	44
30	Quantum Mechanical Investigations on the Formation of Complex Organic Molecules on Interstellar Ice Mantles. Review and Perspectives. ACS Earth and Space Chemistry, 2019, 3, 1499-1523.	1.2	41
31	Accretion of Water in Carbonaceous Chondrites: Current Evidence and Implications for the Delivery of Water to Early Earth. Space Science Reviews, 2019, 215, 1.	3.7	41
32	Ab initio modeling of protein/biomaterial interactions: competitive adsorption between glycine and water onto hydroxyapatite surfaces. Physical Chemistry Chemical Physics, 2009, 11, 9005.	1.3	40
33	Palladium Nanoparticles Entrapped in Heavily Fluorinated Compounds. Chemistry of Materials, 2006, 18, 716-722.	3.2	38
34	Toward a Surface Science Model for Biology: Glycine Adsorption on Nanohydroxyapatite with Well-Defined Surfaces. Journal of Physical Chemistry Letters, 2011, 2, 1390-1394.	2.1	38
35	Glycine Adsorption at Nonstoichiometric (010) Hydroxyapatite Surfaces: A B3LYP Study. Journal of Physical Chemistry C, 2012, 116, 14561-14567.	1.5	36
36	Formation of hydroxyacetonitrile (HOCH₂CN) and polyoxymethylene (POM)-derivatives in comets from formaldehyde (CH₂O) and hydrogen cyanide (HCN) activated by water. Physical Chemistry Chemical Physics, 2014, 16, 3360-3370.	1.3	36

#	Article	IF	Citations
37	Radical recombination in interstellar ices, a not so simple mechanism. Physical Chemistry Chemical Physics, 2017, 19, 2857-2866.	1.3	36
38	Chemical Desorption versus Energy Dissipation: Insights from Ab Initio Molecular Dynamics of HCOÂ· Formation. Astrophysical Journal, 2020, 897, 56.	1.6	36
39	Peptide bond formation activated by the interplay of Lewis and BrÃ¸nsted catalysts. Chemical Physics Letters, 2005, 408, 295-301.	1.2	35
40	Coordination properties of glycylglycine to Cu+, Ni+ and Co+. Influence of metal cation electronic configuration. New Journal of Chemistry, 2005, 29, 1585.	1.4	32
41	Is the Peptide Bond Formation Activated by Cu2+Interactions? Insights from Density Functional Calculations. Journal of Physical Chemistry B, 2007, 111, 5740-5747.	1.2	32
42	Ab initio modelling of proteinâ€“biomaterial interactions: influence of amino acid polar side chains on adsorption at hydroxyapatite surfaces. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 1478-1498.	1.6	30
43	Physisorption vs. chemisorption of probe molecules on boron nitride nanomaterials: the effect of surface curvature. Physical Chemistry Chemical Physics, 2013, 15, 13190.	1.3	30
44	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.	1.5	30
45	Interstellar H adsorption and H₂formation on the crystalline (010) forsterite surface: a B3LYP-D2* periodic study. Physical Chemistry Chemical Physics, 2014, 16, 17447-17457.	1.3	28
46	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.	1.5	28
47	Seeds of Life in Space (SOLIS). III. Zooming Into the Methanol Peak of the Prestellar Core L1544*. Astrophysical Journal, 2018, 855, 112.	1.6	28
48	Water Adsorption on MO₂ (M = Ti, Ru, and Ir) Surfaces. Importance of Octahedral Distortion and Cooperative Effects. ACS Omega, 2019, 4, 2989-2999.	1.6	28
49	FAUST I. The hot corino at the heart of the prototypical Class I protostar L1551 IRS5. Monthly Notices of the Royal Astronomical Society: Letters, 2020, 498, L87-L92.	1.2	27
50	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.	1.1	26
51	IR spectral fingerprint of carbon monoxide in interstellar waterâ€“ice models. Monthly Notices of the Royal Astronomical Society, 2018, 480, 1427-1444.	1.6	26
52	H₂ Formation on Interstellar Grains and the Fate of Reaction Energy. Astrophysical Journal, 2021, 917, 49.	1.6	26
53	Revisiting the reactivity between HCO and CH3 on interstellar grain surfaces. Monthly Notices of the Royal Astronomical Society, 2020, 493, 2523-2527.	1.6	25
54	Gas phase reactivity of Cu+-aromatic amino acids. International Journal of Mass Spectrometry, 2006, 257, 60-69.	0.7	24

#	Article	IF	Citations
55	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.	1.8	24
56	FORMALDEHYDE CHEMISTRY IN COMETARY ICES: ON THE PROSPECTIVE DETECTION OF NH₂CH₂OH, HOCH₂OH, AND POM BY THE ON-BOARD ROSINA INSTRUMENT OF THEROSETTAMISSION. Astrophysical Journal, 2014, 791, 75.	1.6	24
57	Quantum Mechanical Simulations of the Radicalâ€“Radical Chemistry on Icy Surfaces. Astrophysical Journal, Supplement Series, 2022, 259, 39.	3.0	24
58	Relevance of silicate surface morphology in interstellar H₂formation. Insights from quantum chemical calculations. Monthly Notices of the Royal Astronomical Society, 2015, 453, 914-924.	1.6	23
59	When the Surface Matters: Prebiotic Peptideâ€Bond Formation on the TiO₂ (101) Anatase Surface through Periodic DFTâ€Ð2 Simulations. Chemistry - A European Journal, 2018, 24, 16292-16301.	1.7	23
60	Influence of Defects in Boron Nitride Nanotubes in the Adsorption of Molecules. Insights from B3LYP-D2* Periodic Simulations. Crystals, 2016, 6, 63.	1.0	22
61	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.	2.2	22
62	Silicate-mediated interstellar water formation: a theoretical study. Monthly Notices of the Royal Astronomical Society, 2019, 482, 5389-5400.	1.6	22
63	Seeds of Life in Space (SOLIS). Astronomy and Astrophysics, 2020, 637, A63.	2.1	22
64	The role of defective silica surfaces in exogenous delivery of prebiotic compounds: clues from first principles calculations. Physical Chemistry Chemical Physics, 2009, 11, 2497.	1.3	21
65	Trapping in water â€“ an important prerequisite for complex reactivity in astrophysical ices: the case of acetone (CH3)2CÂ=ÂO and ammonia NH3. Monthly Notices of the Royal Astronomical Society, 2014, 443, 2991-3000.	1.6	21
66	Formaldehyde chemistry in cometary ices: the case of HOCH₂OH formation. Physical Chemistry Chemical Physics, 2014, 16, 24200-24208.	1.3	21
67	Forsterite Surfaces as Models of Interstellar Core Dust Grains: Computational Study of Carbon Monoxide Adsorption. ACS Earth and Space Chemistry, 2017, 1, 384-398.	1.2	21
68	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
69	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.	1.1	20
70	Binding Properties of Cu^{+/2+}-(glycyl)_nglycine Complexes (n =) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.1	19
71	Search and Characterization of Transition State Structures in Crystalline Systems Using Valence Coordinates. Journal of Chemical Theory and Computation, 2010, 6, 1341-1350.	2.3	19
72	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.	1.2	19

#	Article	IF	Citations
73	FAUST. II. Discovery of a Secondary Outflow in IRAS 15398â^'3359: Variability in Outflow Direction during the Earliest Stage of Star Formation?. Astrophysical Journal, 2021, 910, 11.	1.6	19
74	Non-energetic Formation of Ethanol via CCH Reaction with Interstellar H₂O Ices. A Computational Chemistry Study. ACS Earth and Space Chemistry, 2022, 6, 496-511.	1.2	19
75	A Theoretical Study on PdII Complexes Containing Hemilabile Pyrazole-Derived Ligands. European Journal of Inorganic Chemistry, 2006, 2006, 447-454.	1.0	18
76	Intrinsic Ladders of Affinity for Amino-Acid-Analogues on Boron Nitride Nanomaterials: A B3LYP-D2* Periodic Study. Journal of Physical Chemistry C, 2015, 119, 17707-17717.	1.5	18
77	Theoretical computations on the efficiency of acetaldehyde formation on interstellar icy grains. Astronomy and Astrophysics, 2021, 655, A9.	2.1	18
78	Accurate 3D fireball trajectory and orbit calculation using the 3D-<scp>firetoc</scp> automatic Python code. Monthly Notices of the Royal Astronomical Society, 2021, 504, 4829-4840.	1.6	17
79	Gas-Phase and Microsolvated Glycine Interacting with Boron Nitride Nanotubes. A B3LYP-D2* Periodic Study. Inorganics, 2014, 2, 334-350.	1.2	15
80	Adsorption of Pharmaceuticals onto Smectite Clay Minerals: A Combined Experimental and Theoretical Study. Minerals (Basel, Switzerland), 2021, 11, 62.	0.8	15
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	Ice chemistry of acetaldehyde reveals competitive reactions in the first step of the Strecker synthesis of alanine: formation of HOâ€“CH(CH3)â€“NH2 vs. HOâ€“CH(CH3)â€“CN. Monthly Notices of the Royal Astronomical Society, 2015, 451, 1649-1660.	1.6	13
83	BCN-M: A Free Computational Tool for Generating Wulff-like Nanoparticle Models with Controlled Stoichiometry. Journal of Physical Chemistry C, 2020, 124, 1227-1237.	1.5	13
84	Computational Surface Modelling of Ices and Minerals of Interstellar Interestâ€"Insights and Perspectives. Minerals (Basel, Switzerland), 2021, 11, 26.	0.8	13
85	Tracing the Primordial Chemical Life of Glycine: A Review from Quantum Chemical Simulations. International Journal of Molecular Sciences, 2022, 23, 4252.	1.8	12
86	Luminous efficiency based on FRIPON meteors and limitations of ablation models. Astronomy and Astrophysics, 2021, 650, A159.	2.1	11
87	Study of Fischerâ€“Tropsch-type reactions on chondritic meteorites. Astronomy and Astrophysics, 2021, 650, A160.	2.1	11
88	In silico study of the interstellar prebiotic formation and delivery of glycine. Rendiconti Lincei, 2011, 22, 137-144.	1.0	10
89	Strained ring motif at silica surfaces: A quantum mechanical study of their reactivity towards protic molecules. Computational and Theoretical Chemistry, 2015, 1074, 168-177.	1.1	10
90	A plausible link between the asteroid 21 Lutetia and <scp>CH</scp> carbonaceous chondrites. Meteoritics and Planetary Science, 2016, 51, 1795-1812.	0.7	10

#	Article	IF	Citations
91	Prebiotic Peptide Bond Formation Through Amino Acid Phosphorylation. Insights from Quantum Chemical Simulations. Life, 2019, 9, 75.	1.1	10
92	Coordination of (Glycyl)_nglycine (n= 1â”3) to Co⁺and Co²⁺. Journal of Physical Chemistry A, 2009, 113, 8883-8892.	1.1	9
93	Canonical, deprotonated, or zwitterionic? II. A computational study on amino acid interaction with the TiO₂(110) rutile surface: comparison with the anatase (101) surface. Physical Chemistry Chemical Physics, 2020, 22, 16862-16876.	1.3	8
94	Interaction of organic compounds with chondritic silicate surfaces. Atomistic insights from quantum chemical periodic simulations. Physical Chemistry Chemical Physics, 2017, 19, 18217-18231.	1.3	7
95	Using fireball networks to track more frequent reentries: Falcon 9 upper-stage orbit determination from video recordings. Astrodynamics, 2021, 5, 347-358.	1.5	7
96	Misaligned Rotations of the Envelope, Outflow, and Disks in the Multiple Protostellar System of VLA 1623â€“2417: FAUST. III. Astrophysical Journal, 2022, 927, 54.	1.6	7
97	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.	1.5	6
98	Multiscale Computational Simulation of Amorphous Silicatesâ€™ Structural, Dielectric, and Vibrational Spectroscopic Properties. Minerals (Basel, Switzerland), 2018, 8, 353.	0.8	6
99	Ab Initio Computational Study on Fe2NiP Schreibersite: Bulk and Surface Characterization. ACS Earth and Space Chemistry, 2021, 5, 1741-1751.	1.2	6
100	Nucleobase Stacking at Clay Edges, a Favorable Interaction for RNA/DNA Oligomerization. ACS Earth and Space Chemistry, 2019, 3, 1023-1033.	1.2	5
101	Interaction of HCO+ Cations With Interstellar Negative Grains. Quantum Chemical Investigation and Astrophysical Implications. Frontiers in Astronomy and Space Sciences, 2021, 8, .	1.1	5
102	Luminous efficiency of meteors derived from ablation model after assessment of its range of validity. Astronomy and Astrophysics, 2021, 652, A84.	2.1	5
103	SOLIS. Astronomy and Astrophysics, 2022, 662, A104.	2.1	5
104	Thermal formation of hydroxynitriles, precursors of hydroxyacids in astrophysical ice analogs: Acetone ((CH3)2CO) and hydrogen cyanide (HCN) reactivity. Molecular Astrophysics, 2015, 1, 1-12.	1.7	3
105	Does Processing or Formation of Water Ice Mantles Affect the Capacity of Nanosilicates to Be the Source of Anomalous Microwave Emission?. Frontiers in Astronomy and Space Sciences, 2021, 8, .	1.1	3
106	Seeds of Life in Space (SOLIS). Astronomy and Astrophysics, 2020, 635, A189.	2.1	2
107	Formation of Interstellar Silicate Dust via Nanocluster Aggregation: Insights From Quantum Chemistry Simulations. Frontiers in Astronomy and Space Sciences, 2021, 8, .	1.1	2
108	Atomistic Simulations of Aqueous Alteration Processes of Mafic Silicates in Carbonaceous Chondrites. Thirty Years of Astronomical Discovery With UKIRT, 2017, , 103-127.	0.3	2

#	Article	IF	Citations
109	Energy signature of ton TNT-class impacts: analysis of the 2018 December 22 fireball over Western Pyrenees. Monthly Notices of the Royal Astronomical Society, 2021, 508, 5716-5733.	1.6	2
110	Binding Energies of N-Bearing Astrochemically-Relevant Molecules on Water Interstellar Ice Models. A Computational Study. Lecture Notes in Computer Science, 2020, , 683-692.	1.0	2
111	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.	2.5	2
112	Computational Simulations of Prebiotic Processes. Cellular Origin and Life in Extreme Habitats, 2012, , 345-362.	0.3	1
113	Computational Investigation on the Thermodynamics of H2COâ€‰+â€‰NH2 â† NH2CHOâ€‰+â€‰H on Interstellar Water Ice Surfaces. Lecture Notes in Computer Science, 2021, , 658-666.	1.0	1
114	Ab initio Calculation of Binding Energies of Interstellar Sulphur-Containing Species on Crystalline Water Ice Models. Lecture Notes in Computer Science, 2021, , 608-619.	1.0	1
115	Water Interaction with Fe2NiP Schreibersite (110) Surface: a Quantum Mechanical Atomistic Perspective. Journal of Physical Chemistry C, 2022, 126, 2243-2252.	1.5	1
116	Ground and Low-Lying States of Cu2+â€”H2O. A Difficult Case for Density Functional Methods.. ChemInform, 2004, 35, no.	0.1	0
117	Modelling of biomaterials: molecular recognition at the surfaces of bioactive glasses. Acta Crystallographica Section A: Foundations and Advances, 2009, 65, s4-s4.	0.3	0
118	Insights on the binding of thioflavin derivative markers to amyloid fibril models and AÎ²1-40 fibrils from computational approaches. , 2014, , .		0
119	Formation of Hexamethylenetetramine â€“ Comment. Origins of Life and Evolution of Biospheres, 2017, 47, 215-215.	0.8	0
120	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, .	1.7	0
121	Formamide Dehydration and Condensation on Acidic Montmorillonite: Mechanistic Insights from Ab-Initio Periodic Simulations. Lecture Notes in Computer Science, 2020, , 502-512.	1.0	0
122	A Combined DFT and RRKM-Based Study on the Reactivity of HCO + NH$$_2$$ on Amorphous Water Ice Surface. Lecture Notes in Computer Science, 2020, , 561-566.	1.0	0