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	Water Interaction with Fe2NiP Schreibersite (110) Surface: a Quantum Mechanical Atomistic Perspective. Journal of Physical Chemistry C, 2022, 126, 2243-2252.	1.5	1
2	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
3	Quantum Mechanical Simulations of the Radicalâ€“Radical Chemistry on Icy Surfaces. Astrophysical Journal, Supplement Series, 2022, 259, 39.	3.0	24
4	SOLIS. Astronomy and Astrophysics, 2022, 662, A104.	2.1	5
5	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
6	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
7	Tracing the Primordial Chemical Life of Glycine: A Review from Quantum Chemical Simulations. International Journal of Molecular Sciences, 2022, 23, 4252.	1.8	12
8	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
9	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
10	Adsorption of Pharmaceuticals onto Smectite Clay Minerals: A Combined Experimental and Theoretical Study. Minerals (Basel, Switzerland), 2021, 11, 62.	0.8	15
11	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
12	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
13	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
14	Formation of Interstellar Silicate Dust via Nanocluster Aggregation: Insights From Quantum Chemistry Simulations. Frontiers in Astronomy and Space Sciences, 2021, 8, .	1.1	2
15	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
16	Luminous efficiency based on FRIPON meteors and limitations of ablation models. Astronomy and Astrophysics, 2021, 650, A159.	2.1	11
17	Ab Initio Computational Study on Fe2NiP Schreibersite: Bulk and Surface Characterization. ACS Earth and Space Chemistry, 2021, 5, 1741-1751.	1.2	6
18	Study of Fischerâ€“Tropsch-type reactions on chondritic meteorites. Astronomy and Astrophysics, 2021, 650, A160.	2.1	11

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19	Theoretical computations on the efficiency of acetaldehyde formation on interstellar icy grains. Astronomy and Astrophysics, 2021, 655, A9.	2.1	18
20	H₂ Formation on Interstellar Grains and the Fate of Reaction Energy. Astrophysical Journal, 2021, 917, 49.	1.6	26
21	Luminous efficiency of meteors derived from ablation model after assessment of its range of validity. Astronomy and Astrophysics, 2021, 652, A84.	2.1	5
22	Computational Surface Modelling of Ices and Minerals of Interstellar Interestâ€"Insights and Perspectives. Minerals (Basel, Switzerland), 2021, 11, 26.	0.8	13
23	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
24	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
25	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
26	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
27	Seeds of Life in Space (SOLIS). Astronomy and Astrophysics, 2020, 635, A189.	2.1	2
28	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
29	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
30	Seeds of Life in Space (SOLIS). Astronomy and Astrophysics, 2020, 637, A63.	2.1	22
31	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
32	Chemical Desorption versus Energy Dissipation: Insights from Ab Initio Molecular Dynamics of HCOÂ· Formation. Astrophysical Journal, 2020, 897, 56.	1.6	36
33	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
34	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
35	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
36	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

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37	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
38	Prebiotic Peptide Bond Formation Through Amino Acid Phosphorylation. Insights from Quantum Chemical Simulations. Life, 2019, 9, 75.	1.1	10
39	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
40	Role of Mineral Surfaces in Prebiotic Chemical Evolution. In Silico Quantum Mechanical Studies. Life, 2019, 9, 10.	1.1	44
41	Nucleobase Stacking at Clay Edges, a Favorable Interaction for RNA/DNA Oligomerization. ACS Earth and Space Chemistry, 2019, 3, 1023-1033.	1.2	5
42	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
43	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
44	Silicate-mediated interstellar water formation: a theoretical study. Monthly Notices of the Royal Astronomical Society, 2019, 482, 5389-5400.	1.6	22
45	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
46	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
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	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
49	Multiscale Computational Simulation of Amorphous Silicatesâ€™ Structural, Dielectric, and Vibrational Spectroscopic Properties. Minerals (Basel, Switzerland), 2018, 8, 353.	0.8	6
50	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.	1.7	23
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	Can Formamide Be Formed on Interstellar Ice? An Atomistic Perspective. ACS Earth and Space Chemistry, 2018, 2, 720-734.	1.2	83
53	Formation of Hexamethylenetetramine â€“ Comment. Origins of Life and Evolution of Biospheres, 2017, 47, 215-215.	0.8	0
54	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

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55	Radical recombination in interstellar ices, a not so simple mechanism. Physical Chemistry Chemical Physics, 2017, 19, 2857-2866.	1.3	36
56	Seeds of Life in Space (SOLIS). Astronomy and Astrophysics, 2017, 605, A57.	2.1	54
57	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
58	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
59	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
60	Seeds of Life in Space (SOLIS). Astronomy and Astrophysics, 2017, 605, L3.	2.1	98
61	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
62	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
63	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
64	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
65	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
66	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
67	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
68	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
69	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
70	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
71	Relevance of silicate surface morphology in interstellar H₂formation. Insights from quantum chemical calculations. Monthly Notices of the Royal Astronomical Society, 2015, 453, 914-924.	1.6	23
72	Insights on the binding of thioflavin derivative markers to amyloid fibril models and AÎ²1-40 fibrils from computational approaches. , 2014, , .		0

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73	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
74	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
75	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
76	Formaldehyde chemistry in cometary ices: the case of HOCH₂OH formation. Physical Chemistry Chemical Physics, 2014, 16, 24200-24208.	1.3	21
77	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
78	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
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	Combined quantum chemical and modeling study of CO hydrogenation on water ice. Astronomy and Astrophysics, 2014, 572, A70.	2.1	87
81	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
82	Silica Surface Features and Their Role in the Adsorption of Biomolecules: Computational Modeling and Experiments. Chemical Reviews, 2013, 113, 4216-4313.	23.0	508
83	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
84	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
85	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
86	COMPUTATIONAL STUDY OF INTERSTELLAR GLYCINE FORMATION OCCURRING AT RADICAL SURFACES OF WATER-ICE DUST PARTICLES. Astrophysical Journal, 2012, 754, 24.	1.6	51
87	Computational Simulations of Prebiotic Processes. Cellular Origin and Life in Extreme Habitats, 2012, , 345-362.	0.3	1
88	Glycine Adsorption at Nonstoichiometric (010) Hydroxyapatite Surfaces: A B3LYP Study. Journal of Physical Chemistry C, 2012, 116, 14561-14567.	1.5	36
89	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
90	The mechanism of hexamethylenetetramine (HMT) formation in the solid state at low temperature. Physical Chemistry Chemical Physics, 2012, 14, 12309.	1.3	52

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91	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
92	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
93	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
94	In silico study of the interstellar prebiotic formation and delivery of glycine. Rendiconti Lincei, 2011, 22, 137-144.	1.0	10
95	Crystal structure of thioflavin-T and its binding to amyloid fibrils: insights at the molecular level. Chemical Communications, 2010, 46, 1156.	2.2	78
96	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
97	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
98	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
99	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
100	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
101	Coordination of (Glycyl)_nglycine (n= 1â^'3) to Co⁺and Co²⁺. Journal of Physical Chemistry A, 2009, 113, 8883-8892.	1.1	9
102	Affinity Scale for the Interaction of Amino Acids with Silica Surfaces. Journal of Physical Chemistry C, 2009, 113, 5741-5750.	1.5	105
103	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
104	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
105	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
106	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
107	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
108	A quantum mechanical study of the reactivity of (SiO)2-defective silica surfaces. Journal of Chemical Physics, 2008, 128, 204702.	1.2	45

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109	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
110	Binding Properties of Cu^{+/2+}-(glycyl)_nglycine Complexes (n =) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.1	19
111	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
112	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
113	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
114	Cationâˆ'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
115	Palladium Nanoparticles Entrapped in Heavily Fluorinated Compounds. Chemistry of Materials, 2006, 18, 716-722.	3.2	38
116	Gas phase reactivity of Cu+-aromatic amino acids. International Journal of Mass Spectrometry, 2006, 257, 60-69.	0.7	24
117	A Theoretical Study on PdII Complexes Containing Hemilabile Pyrazole-Derived Ligands. European Journal of Inorganic Chemistry, 2006, 2006, 447-454.	1.0	18
118	Does Silica Surface Catalyse Peptide Bond Formation? New Insights from First-Principles Calculations. ChemPhysChem, 2006, 7, 157-163.	1.0	77
119	Peptide bond formation activated by the interplay of Lewis and BrÃ¸nsted catalysts. Chemical Physics Letters, 2005, 408, 295-301.	1.2	35
120	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
121	Ground and Low-Lying States of Cu2+â€"H2O. A Difficult Case for Density Functional Methods.. ChemInform, 2004, 35, no.	0.1	0
122	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