Piero Ugliengo

List of Publications by Year
in descending order

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269	11,967	25034	39675
papers	citations	57 h-index	94 g-index

279	279	279	8935
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	B3LYP augmented with an empirical dispersion term (B3LYP-D*) as applied to molecular crystals. CrystEngComm, 2008, 10, 405-410.	2.6	775
2	Theoretical Study of van der Waals Complexes at Surface Sites in Comparison with the Experiment. Chemical Reviews, 1994, 94, 2095-2160.	47.7	704
3	Silica Surface Features and Their Role in the Adsorption of Biomolecules: Computational Modeling and Experiments. Chemical Reviews, 2013, 113, 4216-4313.	47.7	508
4	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
5	Intermolecular Interaction Energies in Molecular Crystals: Comparison and Agreement of Localized MÃ¸llerâ€“Plesset 2, Dispersion-Corrected Density Functional, and Classical Empirical Two-Body Calculations. Journal of Physical Chemistry A, 2011, 115, 11179-11186.	2.5	169
6	Title is missing!. Topics in Catalysis, 2001, 15, 43-52.	2.8	159
7	Experimental and Quantum Chemical Studies on the Adsorption of Carbon Dioxide on Alkali-Metal-Exchanged ZSM-5 Zeolites. Journal of Physical Chemistry B, 2000, 104, 10978-10988.	2.6	156
8	Periodic ab initio study of structural and vibrational features of hexagonal hydroxyapatite Ca10(PO4)6(OH)2. Physical Chemistry Chemical Physics, 2006, 8, 2464.	2.8	153
9	MOLDRAW: Molecular graphics on a personal computer. Zeitschrift Fur Kristallographie - Crystalline Materials, 1993, 207, 9-23.	0.8	142
10	Vibrational spectrum of brucite, Mg(OH)2: a periodic ab initio quantum mechanical calculation including OH anharmonicity. Chemical Physics Letters, 2004, 396, 308-315.	2.6	142
11	Vibration Frequencies of Mg3Al2Si3O12 Pyrope. An ab Initio Study with the CRYSTAL Code. Journal of Physical Chemistry B, 2005, 109, 6146-6152.	2.6	142
12	Hydroxyapatite as a key biomaterial: quantum-mechanical simulation of its surfaces in interaction with biomolecules. Physical Chemistry Chemical Physics, 2010, 12, 6309.	2.8	136
13	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.	4.5	116
14	Ab initio study of the adducts of carbon monoxide with alkaline cations. Journal of Chemical Physics, 1996, 105, 4129-4139.	3.0	114
15	Performance of six functionals (LDA, PBE, PBESOL, B3LYP, PBE0, and WC1LYP) in the simulation of vibrational and dielectric properties of crystalline compounds. The case of forsterite Mg₂SiO₄. Journal of Computational Chemistry, 2011, 32, 1775-1784.	3.3	112
16	Characterisation of defective silicalitesâ€Šâ€. Dalton Transactions RSC, 2000, , 3921-3929.	2.3	108
17	Affinity Scale for the Interaction of Amino Acids with Silica Surfaces. Journal of Physical Chemistry C, 2009, 113, 5741-5750.	3.1	105
18	Structural and induced heterogeneity at the surface of some silica polymorphs from the enthalpy of adsorption of various molecules. Langmuir, 1993, 9, 2712-2720.	3.5	103

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19	Seeds of Life in Space (SOLIS). Astronomy and Astrophysics, 2017, 605, L3.	5.1	98
20	Ab Initio Modeling of Protein/Biomaterial Interactions: Glycine Adsorption at Hydroxyapatite Surfaces. Journal of the American Chemical Society, 2008, 130, 16181-16183.	13.7	97
21	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
22	Quantum mechanical calculation of the OH vibrational frequency in crystalline solids. Molecular Physics, 2005, 103, 2549-2558.	1.7	93
23	Thermodynamic Study of Water Adsorption in High-Silica Zeolites. Journal of Physical Chemistry B, 2006, 110, 14849-14859.	2.6	93
24	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
25	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
26	J-ICE: a newJmolinterface for handling and visualizing crystallographic and electronic properties. Journal of Applied Crystallography, 2011, 44, 225-229.	4.5	88
27	Combined quantum chemical and modeling study of CO hydrogenation on water ice. Astronomy and Astrophysics, 2014, 572, A70.	5.1	87
28	Assessment of Different Quantum Mechanical Methods for the Prediction of Structure and Cohesive Energy of Molecular Crystals. Journal of Chemical Theory and Computation, 2016, 12, 3340-3352.	5.3	85
29	Cation Selectivity in Alkali-Exchanged Chabazite:Â An ab Initio Periodic Study. Chemistry of Materials, 2003, 15, 3996-4004.	6.7	83
30	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
31	Can Formamide Be Formed on Interstellar Ice? An Atomistic Perspective. ACS Earth and Space Chemistry, 2018, 2, 720-734.	2.7	83
32	Water Adsorption on the Stoichiometric (001) and (010) Surfaces of Hydroxyapatite: A Periodic B3LYP Study. Langmuir, 2009, 25, 2188-2198.	3.5	80
33	Crystal structure of thioflavin-T and its binding to amyloid fibrils: insights at the molecular level. Chemical Communications, 2010, 46, 1156.	4.1	78
34	Does Silica Surface Catalyse Peptide Bond Formation? New Insights from First-Principles Calculations. ChemPhysChem, 2006, 7, 157-163.	2.1	77
35	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
36	Nearly free surface silanols are the critical molecular moieties that initiate the toxicity of silica particles. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 27836-27846.	7.1	76

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37	First Principles Calculations of the Adsorption of NH3on a Periodic Model of the Silica Surface. Journal of Physical Chemistry B, 2000, 104, 9491-9499.	2.6	75
38	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
39	Role of dispersive interactions in layered materials: a periodic B3LYP and B3LYP-D* study of Mg(OH)2, Ca(OH)2 and kaolinite. Journal of Materials Chemistry, 2009, 19, 2564.	6.7	75
40	A periodic ab initio study of the structure and relative stability of silica polymorphs. Chemical Physics Letters, 1998, 292, 394-402.	2.6	74
41	Quantum Mechanical ab Initio Characterization of a Simple Periodic Model of the Silica Surface. Journal of Physical Chemistry B, 1999, 103, 2165-2171.	2.6	74
42	Ab initio study of HCl and HF interaction with crystalline ice. I. Physical adsorption. Journal of Chemical Physics, 1998, 108, 9516-9528.	3.0	72
43	A comparison between plane wave and Gaussian-type orbital basis sets for hydrogen bonded systems: Formic acid as a test case. Journal of Chemical Physics, 2007, 127, 154102.	3.0	72
44	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
45	Does Dispersion Dominate over H-Bonds in Drugâ€“Surface Interactions? The Case of Silica-Based Materials As Excipients and Drug-Delivery Agents. Journal of Chemical Theory and Computation, 2013, 9, 2404-2415.	5.3	72
46	Hydrogen Bond in Layered Materials:Â Structural and Vibrational Properties of Kaolinite by a Periodic B3LYP Approach. Chemistry of Materials, 2006, 18, 2135-2143.	6.7	70
47	Calorimetric and IR spectroscopic study of the interaction of NH3 with variously prepared defective silicalites. Applied Surface Science, 2002, 196, 56-70.	6.1	68
48	Infrared Spectra of Hydrogen-Bonded Ionic Crystals:Â Ab Initio Study of Mg(OH)2and Î²-Be(OH)2. Journal of Physical Chemistry B, 2004, 108, 13632-13637.	2.6	68
49	FFSiOH: a New Force Field for Silica Polymorphs and Their Hydroxylated Surfaces Based on Periodic B3LYP Calculations. Chemistry of Materials, 2008, 20, 2522-2531.	6.7	68
50	Proton-ordered models of ordinary ice for quantum-mechanical studies. Journal of Chemical Physics, 1997, 106, 8030-8040.	3.0	67
51	Proton-ordered ice structures at zero pressure. A quantum-mechanical investigation. Chemical Physics Letters, 1996, 253, 201-208.	2.6	66
52	Superoxide ions formed on MgO through the agency of presorbed molecules. Part 1.â€”Spectroscopic electron spin resonance features. Journal of the Chemical Society Faraday Transactions I, 1989, 85, 1373.	1.0	65
53	Structure and vibrational spectra of crystalline SiO2 ultra-thin films on Mo(112). Surface Science, 2005, 584, 225-236.	1.9	65
54	Binding Energies of Interstellar Molecules on Crystalline and Amorphous Models of Water Ice by Ab Initio Calculations. Astrophysical Journal, 2020, 904, 11.	4.5	65

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55	Temkin-type model for the description of induced heterogeneity: CO adsorption on Group 4 transition metal dioxides. Langmuir, 1993, 9, 1521-1528.	3.5	63
56	Quantum Chemical Calculations and Experimental Evidence for O-Bonding of Carbon Monoxide to Alkali Metal Cations in Zeolites. Journal of Physical Chemistry B, 1999, 103, 4839-4846.	2.6	60
57	Role of dispersive interactions in the CO adsorption on MgO(001): periodic B3LYP calculations augmented with an empirical dispersion term. Physical Chemistry Chemical Physics, 2010, 12, 6382.	2.8	60
58	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.	2.8	60
59	Ab Initio Study of the Adducts of Small Molecules with the Isolated Hydroxyl of Silica and the BrÃ¸nsted Site in Zeolites:â€‰ A Comparison between B3-LYP and MP2 Methods. Journal of Physical Chemistry B, 1998, 102, 2373-2382.	2.6	55
60	The vibrational features of hydroxylapatite and type A carbonated apatite: A first principle contribution. American Mineralogist, 2013, 98, 752-759.	1.9	55
61	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.	2.7	55
62	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.	2.7	55
63	Modeling physisorption with the ONIOM method: the case of NH3 at the isolated hydroxyl group of the silica surface. Chemical Physics Letters, 2001, 341, 625-632.	2.6	54
64	Are dispersive forces relevant for CO adsorption on the MgO(001) surface?. Chemical Physics Letters, 2002, 366, 683-690.	2.6	54
65	Characterisation of Lewis and BrÃ¸nsted acidic sites in H-MFI and H-BEA zeolites: a thermodynamic and ab initio study. Thermochimica Acta, 2004, 418, 3-9.	2.7	54
66	The structural, electronic and vibrational properties of LiOH and NaOH: an ab initio study. Chemical Physics Letters, 2004, 387, 453-459.	2.6	54
67	Ab initio quantum mechanical study of Î³-AlOOH boehmite: structure and vibrational spectrum. Physics and Chemistry of Minerals, 2009, 36, 47-59.	0.8	54
68	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
69	Seeds of Life in Space (SOLIS). Astronomy and Astrophysics, 2017, 605, A57.	5.1	54
70	Reactions of silica strained rings: an experimental and ab-initio study. Surface Science, 1995, 323, 151-162.	1.9	53
71	Vibrational Spectrum of Katoite Ca3Al2[(OH)4]3:Â A Periodic ab Initio Study. Journal of Physical Chemistry B, 2006, 110, 692-701.	2.6	53
72	H-Chabazite with variable Si/Al ratio: stability and OH vibrational frequency computed in a periodic LCAO B3-LYP approach. Chemical Physics Letters, 2000, 318, 247-255.	2.6	52

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73	Large-Scale B3LYP Simulations of Ibuprofen Adsorbed in MCM-41 Mesoporous Silica as Drug Delivery System. Journal of Physical Chemistry C, 2014, 118, 26737-26749.	3.1	52
74	A Nanostructured Porous Silicon Near Insulator Becomes Either a p- or an n-Type Semiconductor upon Gas Adsorption. Advanced Materials, 2005, 17, 528-531.	21.0	51
75	COMPUTATIONAL STUDY OF INTERSTELLAR GLYCINE FORMATION OCCURRING AT RADICAL SURFACES OF WATER-ICE DUST PARTICLES. Astrophysical Journal, 2012, 754, 24.	4.5	51
76	Does Adsorption at Hydroxyapatite Surfaces Induce Peptide Folding? Insights from Large-Scale B3LYP Calculations. Journal of the American Chemical Society, 2012, 134, 10899-10910.	13.7	51
77	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
78	Ammonia and water as probes for the surface reactivity of covalent solids: cristobalite and silicon carbide. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 277.	1.7	50
79	Methylation of phenol over high-silica beta zeolite: Effect of zeolite acidity and crystal size on catalyst behaviour. Journal of Catalysis, 2007, 245, 285-300.	6.2	50
80	Physico-Chemical Features of Aluminum Hydroxides As Modeled with the Hybrid B3LYP Functional and Localized Basis Functions. Journal of Physical Chemistry C, 2011, 115, 13107-13134.	3.1	50
81	Vibrational modes of isolated hydroxyls of silica computed ab initio in a cluster approach. Chemical Physics Letters, 1998, 294, 103-108.	2.6	49
82	CO/MgO(001) at different CO coverages: a periodic ab initio Hartreeâ€“Fock and B3-LYP study. Surface Science, 2001, 479, 255-272.	1.9	48
83	Coordination chemistry of Ca sites at the surface of nanosized hydroxyapatite: interaction with H ₂ O and CO. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 1313-1336.	3.4	48
84	Neutral vs Zwitterionic Glycine Forms at the Water/Silica Interface: Structure, Energies, and Vibrational Features from B3LYP Periodic Simulations. Langmuir, 2008, 24, 14027-14034.	3.5	47
85	Atomistic Model of Micelle-Templated Mesoporous Silicas: Structural, Morphological, and Adsorption Properties. Langmuir, 2012, 28, 11131-11141.	3.5	47
86	Silica-Based Materials as Drug Adsorbents: First Principle Investigation on the Role of Water Microsolvation on Ibuprofen Adsorption. Journal of Physical Chemistry A, 2014, 118, 5801-5807.	2.5	47
87	Induced heterogeneity at the surface of group 4 dioxides as revealed by CO adsorption at room temperature. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 391.	1.7	45
88	A quantum mechanical study of the reactivity of (SiO)2-defective silica surfaces. Journal of Chemical Physics, 2008, 128, 204702.	3.0	45
89	Hydrogarnet defect in chabazite and sodalite zeolites: A periodic Hartreeâ€“Fock and B3-LYP study. Journal of Chemical Physics, 2002, 117, 5337-5346.	3.0	44
90	Role of Mineral Surfaces in Prebiotic Chemical Evolution. In Silico Quantum Mechanical Studies. Life, 2019, 9, 10.	2.4	44

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91	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
92	Synthesis and Structural Investigation of Zr(BH₄)₄. Journal of Physical Chemistry C, 2012, 116, 20239-20245.	3.1	43
93	A new massively parallel version of CRYSTAL for large systems on high performance computing architectures. Journal of Computational Chemistry, 2012, 33, 2276-2284.	3.3	43
94	B3LYP Simulation of the Full Vibrational Spectrum of 45S5 Bioactive Silicate Glass Compared to ν-Silica. Chemistry of Materials, 2008, 20, 5610-5621.	6.7	42
95	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.	2.7	41
96	Experimental evidence for the hyperfine interaction between a surface superoxide species on MgO and a neighbouring hydroxylic proton. Journal of the Chemical Society Faraday Transactions I, 1989, 85, 3987.	1.0	40
97	Structure and Energetics of SiO2Polymorphs by Quantum-Mechanical and Semiclassical Approaches. Journal of Physical Chemistry B, 2000, 104, 7259-7265.	2.6	40
98	Ab initio modeling of protein/biomaterial interactions: competitive adsorption between glycine and water onto hydroxyapatite surfaces. Physical Chemistry Chemical Physics, 2009, 11, 9005.	2.8	40
99	Vibrational Properties of MBH₄ and MBF₄ Crystals (M = Li, Na, K): A Combined DFT, Infrared, and Raman Study. Journal of Physical Chemistry C, 2011, 115, 18890-18900.	3.1	39
100	Toward a Surface Science Model for Biology: Glycine Adsorption on Nanohydroxyapatite with Well-Defined Surfaces. Journal of Physical Chemistry Letters, 2011, 2, 1390-1394.	4.6	38
101	Elastic and Vibrational Properties of Î±- and Î²-PbO.. Journal of Physical Chemistry C, 2012, 116, 21514-21522.	3.1	38
102	The Surface of Ordered Mesoporous Benzeneâ€'Silica Hybrid Material:â€‰ An Infrared and ab Initio Molecular Modeling Study. Journal of Physical Chemistry B, 2005, 109, 11961-11966.	2.6	36
103	A computational study on the effect of fluorine substitution in LiBH4. Journal of Alloys and Compounds, 2011, 509, S679-S683.	5.5	36
104	Stability of the Dipolar (001) Surface of Hydroxyapatite. Journal of Physical Chemistry C, 2012, 116, 6108-6114.	3.1	36
105	Glycine Adsorption at Nonstoichiometric (010) Hydroxyapatite Surfaces: A B3LYP Study. Journal of Physical Chemistry C, 2012, 116, 14561-14567.	3.1	36
106	Chemical Desorption versus Energy Dissipation: Insights from Ab Initio Molecular Dynamics of HCOÂ· Formation. Astrophysical Journal, 2020, 897, 56.	4.5	36
107	Density functional study of hydrogen-bonded systems: Energetic and vibrational features of some gas-phase adducts of hydrogen fluoride. Computational and Theoretical Chemistry, 1997, 419, 227-238.	1.5	35
108	Peptide bond formation activated by the interplay of Lewis and BrÃ¸nsted catalysts. Chemical Physics Letters, 2005, 408, 295-301.	2.6	35

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109	Periodic ab initio bulk investigation of hydroxylapatite and type A carbonated apatite with both pseudopotential and all-electron basis sets for calcium atoms. American Mineralogist, 2013, 98, 410-416.	1.9	35
110	DFT investigation of structural and vibrational properties of type B and mixed A-B carbonated hydroxylapatite. American Mineralogist, 2014, 99, 117-127.	1.9	35
111	Exfoliation Energy of Layered Materials by DFT-D: Beware of Dispersion!. Journal of Chemical Theory and Computation, 2020, 16, 5244-5252.	5.3	35
112	Relative propensity of methanol and silanol towards hydrogen bond formation. Chemical Physics Letters, 1992, 191, 537-547.	2.6	34
113	Periodic B3LYP study of hydroxyapatite (001) surface modelled by thin layer slabs. European Journal of Mineralogy, 2007, 19, 757-767.	1.3	34
114	Theoretical Study of Molecular Hydrogen Adsorption in Mg-Exchanged Chabazite. Journal of Physical Chemistry C, 2007, 111, 1871-1873.	3.1	34
115	Functionalization of Zeolitic Cavities:â€‰ Grafting NH₂ Groups in Framework T Sites of B-SSZ-13 A Way to Obtain Basic Solids Catalysts?. Journal of the American Chemical Society, 2007, 129, 12131-12140.	13.7	34
116	MOLDRAW: Molecular graphics on a personal computer. Zeitschrift Fur Kristallographie - Crystalline Materials, 1993, 208, 383-383.	0.8	33
117	Cage-like clusters as models for the hydroxyls of silica: ab initio calculation of 1H and 29Si NMR chemical shifts. Chemical Physics Letters, 1999, 299, 443-450.	2.6	33
118	Silanol as a model for the free hydroxyl of amorphous silica: comparison between experimental and calculated ab initio vibrational features. Journal of Molecular Catalysis, 1989, 54, 439-443.	1.2	32
119	Carbon monoxide adsorption on alkali and proton-exchanged chabazite: anab-initioperiodic study using the CRYSTAL code. Molecular Physics, 2005, 103, 2559-2571.	1.7	32
120	An ab initio parameterized interatomic force field for hydroxyapatite. Journal of Materials Chemistry, 2007, 17, 2061.	6.7	32
121	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
122	A computational multiscale strategy to the study of amorphous materials. Theoretical Chemistry Accounts, 2007, 117, 933-942.	1.4	32
123	Periodic B3-LYP calculations on H-Edingtonites, both alone and interacting with acetylene. Physical Chemistry Chemical Physics, 1999, 1, 545-553.	2.8	31
124	How Does Collagen Adsorb on Hydroxyapatite? Insights From Ab Initio Simulations on a Polyproline Type II Model. Journal of Physical Chemistry C, 2019, 123, 7540-7550.	3.1	31
125	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.	3.4	30
126	Theoretical and Experimental Study of LiBH4-LiCl Solid Solution. Crystals, 2012, 2, 144-158.	2.2	30

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127	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
128	Stereospecific synthesis of squalenoid epoxide vinyl ethers as inhibitors of 2,3-oxidosqualene cyclase. Journal of the Chemical Society Perkin Transactions 1, 1988, , 461-469.	0.9	29
129	Infrared Spectroscopy Study of the Adsorption of Carbonyl Compounds on Severely Outgassed Silica: Spectroscopic and Thermodynamic Results. Langmuir, 1995, 11, 4811-4817.	3.5	29
130	VitaminC at 120K: experimental and theoretical study of the charge density. Computational and Theoretical Chemistry, 1997, 419, 139-154.	1.5	29
131	Surface Properties of Silica-Based Biomaterials: Ca Species at the Surface of Amorphous Silica As Model Sites. Journal of Physical Chemistry C, 2008, 112, 16879-16892.	3.1	29
132	Water at hydroxyapatite surfaces: the effect of coverage and surface termination as investigated by all-electron B3LYP-D* simulations. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	29
133	IR Study of the Adsorption of Unsaturated Hydrocarbons on Highly Outgassed Silica:â€‰ Spectroscopic and Thermodynamic Results. Langmuir, 1997, 13, 5107-5113.	3.5	28
134	Molecular Water on Exposed Al3+ Cations Is a Source of Acidity in Silicoaluminas. Journal of Physical Chemistry B, 2006, 110, 19087-19092.	2.6	28
135	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
136	Seeds of Life in Space (SOLIS). III. Zooming Into the Methanol Peak of the Prestellar Core L1544*. Astrophysical Journal, 2018, 855, 112.	4.5	28
137	Periodic DFT Study of Radical Species on Crystalline Silica Surfaces. Journal of Physical Chemistry C, 2010, 114, 16430-16438.	3.1	27
138	Affinity of hydroxyapatite (001) and (010) surfaces to formic and alendronic acids: a quantum-mechanical and infrared study. Physical Chemistry Chemical Physics, 2011, 13, 1099-1111.	2.8	27
139	Simulation and Experiment Reveal a Complex Scenario for the Adsorption of an Antifungal Drug in Ordered Mesoporous Silica. Journal of Physical Chemistry C, 2015, 119, 13068-13079.	3.1	27
140	Comparison of different approaches to the study of local defects in crystals. I. Theoretical considerations and computational schemes. Physica Status Solidi (B): Basic Research, 1983, 116, 249-259.	1.5	26
141	Ab initio study of the gas-phase equilibrium between (H2O)4 and (H2O)8. Chemical Physics Letters, 1993, 212, 644-648.	2.6	26
142	IR spectral fingerprint of carbon monoxide in interstellar waterâ€“ice models. Monthly Notices of the Royal Astronomical Society, 2018, 480, 1427-1444.	4.4	26
143	H₂ Formation on Interstellar Grains and the Fate of Reaction Energy. Astrophysical Journal, 2021, 917, 49.	4.5	26
144	Bi-dimensional CO clusters at the surface of polycrystalline monoclinic ZrO2. Materials Chemistry and Physics, 1991, 29, 457-466.	4.0	25

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145	Cagelike Clusters as Models for the Isolated Hydroxyls of Silica:ÂAb InitioB3-LYP Calculations of the Interaction with Ammoniaâ€. Langmuir, 1999, 15, 5829-5835.	3.5	25
146	FTIR spectroscopic and ab initio evidence for an amphipathic character of CO bonding with silanol groups. Chemical Physics Letters, 2003, 374, 439-445.	2.6	25
147	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
148	Revisiting the reactivity between HCO and CH3 on interstellar grain surfaces. Monthly Notices of the Royal Astronomical Society, 2020, 493, 2523-2527.	4.4	25
149	Ab InitioConformational Study of the Phenylisoserine Side Chain of Paclitaxel. Journal of Medicinal Chemistry, 1999, 42, 291-299.	6.4	24
150	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
151	Quantum Mechanical Simulations of the Radicalâ€“Radical Chemistry on Icy Surfaces. Astrophysical Journal, Supplement Series, 2022, 259, 39.	7.7	24
152	Structural, electronic, and vibrational properties of solid Sr(OH)2, calculated with different Hamiltonians. Journal of Chemical Physics, 2003, 119, 1045-1052.	3.0	23
153	An Ab Initio Periodic Study of Acidic Chabazite as a Candidate for Dihydrogen Storage. Journal of Physical Chemistry B, 2006, 110, 10467-10474.	2.6	23
154	Hydrophobic Behavior of Dehydroxylated Silica Surfaces: A B3LYP Periodic Study. Journal of Physical Chemistry C, 2010, 114, 19984-19992.	3.1	23
155	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
156	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.	3.3	23
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