

Piero Ugliengo

List of Publications by Year in descending order

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269
papers

11,967
citations

24978

57
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39575

94
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279
all docs

279
docs citations

279
times ranked

8935
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.	1.3	775
2	Theoretical Study of van der Waals Complexes at Surface Sites in Comparison with the Experiment. Chemical Reviews, 1994, 94, 2095-2160.	23.0	704
3	Silica Surface Features and Their Role in the Adsorption of Biomolecules: Computational Modeling and Experiments. Chemical Reviews, 2013, 113, 4216-4313.	23.0	508
4	Realistic Models of Hydroxylated Amorphous Silica Surfaces and MCM-41 Mesoporous Material Simulated by Large-scale Periodic B3LYP Calculations. Advanced Materials, 2008, 20, 4579-4583.	11.1	199
5	Intermolecular Interaction Energies in Molecular Crystals: Comparison and Agreement of Localized Møller-Plesset 2, Dispersion-Corrected Density Functional, and Classical Empirical Two-Body Calculations. Journal of Physical Chemistry A, 2011, 115, 11179-11186.	1.1	169
6	Title is missing!. Topics in Catalysis, 2001, 15, 43-52.	1.3	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.	1.2	156
8	Periodic ab initio study of structural and vibrational features of hexagonal hydroxyapatite Ca ₁₀ (PO ₄) ₆ (OH) ₂ . Physical Chemistry Chemical Physics, 2006, 8, 2464.	1.3	153
9	MOLDRAW: Molecular graphics on a personal computer. Zeitschrift Fur Kristallographie - Crystalline Materials, 1993, 207, 9-23.	0.4	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.	1.2	142
11	Vibration Frequencies of Mg ₃ Al ₂ Si ₃ O ₁₂ Pyrope. An ab Initio Study with the CRYSTAL Code. Journal of Physical Chemistry B, 2005, 109, 6146-6152.	1.2	142
12	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
13	Seeds Of Life In Space (SOLIS): The Organic Composition Diversity at 300-1000 au Scale in Solar-type Star-forming Regions. Astrophysical Journal, 2017, 850, 176.	1.6	116
14	Ab initio study of the adducts of carbon monoxide with alkaline cations. Journal of Chemical Physics, 1996, 105, 4129-4139.	1.2	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 Mg ₂ SiO ₄ . Journal of Computational Chemistry, 2011, 32, 1775-1784.	1.5	112
16	Characterisation of defective silicalites. 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.	1.5	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.	1.6	103

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19	Seeds of Life in Space (SOLIS). <i>Astronomy and Astrophysics</i> , 2017, 605, L3.	2.1	98
20	Ab Initio Modeling of Protein/Biomaterial Interactions: Glycine Adsorption at Hydroxyapatite Surfaces. <i>Journal of the American Chemical Society</i> , 2008, 130, 16181-16183.	6.6	97
21	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
22	Quantum mechanical calculation of the OH vibrational frequency in crystalline solids. <i>Molecular Physics</i> , 2005, 103, 2549-2558.	0.8	93
23	Thermodynamic Study of Water Adsorption in High-Silica Zeolites. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14849-14859.	1.2	93
24	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
25	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
26	JHCE: a new Jmol interface for handling and visualizing crystallographic and electronic properties. <i>Journal of Applied Crystallography</i> , 2011, 44, 225-229.	1.9	88
27	Combined quantum chemical and modeling study of CO hydrogenation on water ice. <i>Astronomy and Astrophysics</i> , 2014, 572, A70.	2.1	87
28	Assessment of Different Quantum Mechanical Methods for the Prediction of Structure and Cohesive Energy of Molecular Crystals. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3340-3352.	2.3	85
29	Cation Selectivity in Alkali-Exchanged Chabazite: An ab Initio Periodic Study. <i>Chemistry of Materials</i> , 2003, 15, 3996-4004.	3.2	83
30	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
31	Can Formamide Be Formed on Interstellar Ice? An Atomistic Perspective. <i>ACS Earth and Space Chemistry</i> , 2018, 2, 720-734.	1.2	83
32	Water Adsorption on the Stoichiometric (001) and (010) Surfaces of Hydroxyapatite: A Periodic B3LYP Study. <i>Langmuir</i> , 2009, 25, 2188-2198.	1.6	80
33	Crystal structure of thioflavin-T and its binding to amyloid fibrils: insights at the molecular level. <i>Chemical Communications</i> , 2010, 46, 1156.	2.2	78
34	Does Silica Surface Catalyse Peptide Bond Formation? New Insights from First-Principles Calculations. <i>ChemPhysChem</i> , 2006, 7, 157-163.	1.0	77
35	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
36	Nearly free surface silanols are the critical molecular moieties that initiate the toxicity of silica particles. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 27836-27846.	3.3	76

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37	First Principles Calculations of the Adsorption of NH ₃ on a Periodic Model of the Silica Surface. <i>Journal of Physical Chemistry B</i> , 2000, 104, 9491-9499.	1.2	75
38	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
39	Role of dispersive interactions in layered materials: a periodic B3LYP and B3LYP-D* study of Mg(OH) ₂ , Ca(OH) ₂ and kaolinite. <i>Journal of Materials Chemistry</i> , 2009, 19, 2564.	6.7	75
40	A periodic ab initio study of the structure and relative stability of silica polymorphs. <i>Chemical Physics Letters</i> , 1998, 292, 394-402.	1.2	74
41	Quantum Mechanical ab Initio Characterization of a Simple Periodic Model of the Silica Surface. <i>Journal of Physical Chemistry B</i> , 1999, 103, 2165-2171.	1.2	74
42	Ab initio study of HCl and HF interaction with crystalline ice. I. Physical adsorption. <i>Journal of Chemical Physics</i> , 1998, 108, 9516-9528.	1.2	72
43	A comparison between plane wave and Gaussian-type orbital basis sets for hydrogen bonded systems: Formic acid as a test case. <i>Journal of Chemical Physics</i> , 2007, 127, 154102.	1.2	72
44	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
45	Does Dispersion Dominate over H-Bonds in Drug-Surface Interactions? The Case of Silica-Based Materials As Excipients and Drug-Delivery Agents. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2404-2415.	2.3	72
46	Hydrogen Bond in Layered Materials: Structural and Vibrational Properties of Kaolinite by a Periodic B3LYP Approach. <i>Chemistry of Materials</i> , 2006, 18, 2135-2143.	3.2	70
47	Calorimetric and IR spectroscopic study of the interaction of NH ₃ with variously prepared defective silicalites. <i>Applied Surface Science</i> , 2002, 196, 56-70.	3.1	68
48	Infrared Spectra of Hydrogen-Bonded Ionic Crystals: Ab Initio Study of Mg(OH) ₂ and Be(OH) ₂ . <i>Journal of Physical Chemistry B</i> , 2004, 108, 13632-13637.	1.2	68
49	FFSiOH: a New Force Field for Silica Polymorphs and Their Hydroxylated Surfaces Based on Periodic B3LYP Calculations. <i>Chemistry of Materials</i> , 2008, 20, 2522-2531.	3.2	68
50	Proton-ordered models of ordinary ice for quantum-mechanical studies. <i>Journal of Chemical Physics</i> , 1997, 106, 8030-8040.	1.2	67
51	Proton-ordered ice structures at zero pressure. A quantum-mechanical investigation. <i>Chemical Physics Letters</i> , 1996, 253, 201-208.	1.2	66
52	Superoxide ions formed on MgO through the agency of presorbed molecules. Part 1. Spectroscopic electron spin resonance features. <i>Journal of the Chemical Society Faraday Transactions I</i> , 1989, 85, 1373.	1.0	65
53	Structure and vibrational spectra of crystalline SiO ₂ ultra-thin films on Mo(112). <i>Surface Science</i> , 2005, 584, 225-236.	0.8	65
54	Binding Energies of Interstellar Molecules on Crystalline and Amorphous Models of Water Ice by Ab Initio Calculations. <i>Astrophysical Journal</i> , 2020, 904, 11.	1.6	65

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55	Temkin-type model for the description of induced heterogeneity: CO adsorption on Group 4 transition metal dioxides. <i>Langmuir</i> , 1993, 9, 1521-1528.	1.6	63
56	Quantum Chemical Calculations and Experimental Evidence for O-Bonding of Carbon Monoxide to Alkali Metal Cations in Zeolites. <i>Journal of Physical Chemistry B</i> , 1999, 103, 4839-4846.	1.2	60
57	Role of dispersive interactions in the CO adsorption on MgO(001): periodic B3LYP calculations augmented with an empirical dispersion term. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6382.	1.3	60
58	Physisorption of aromatic organic contaminants at the surface of hydrophobic/hydrophilic silica geosorbents: a B3LYP-D modeling study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6357.	1.3	60
59	Ab Initio Study of the Adducts of Small Molecules with the Isolated Hydroxyl of Silica and the Brønsted Site in Zeolites: A Comparison between B3-LYP and MP2 Methods. <i>Journal of Physical Chemistry B</i> , 1998, 102, 2373-2382.	1.2	55
60	The vibrational features of hydroxylapatite and type A carbonated apatite: A first principle contribution. <i>American Mineralogist</i> , 2013, 98, 752-759.	0.9	55
61	Reactivity of HCO with CH ₃ and NH ₂ on Water Ice Surfaces. A Comprehensive Accurate Quantum Chemistry Study. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 2158-2170.	1.2	55
62	Thermal Desorption of Interstellar Ices: A Review on the Controlling Parameters and Their Implications from Snowlines to Chemical Complexity. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 597-630.	1.2	55
63	Modeling physisorption with the ONIOM method: the case of NH ₃ at the isolated hydroxyl group of the silica surface. <i>Chemical Physics Letters</i> , 2001, 341, 625-632.	1.2	54
64	Are dispersive forces relevant for CO adsorption on the MgO(001) surface?. <i>Chemical Physics Letters</i> , 2002, 366, 683-690.	1.2	54
65	Characterisation of Lewis and Brønsted acidic sites in H-MFI and H-BEA zeolites: a thermodynamic and ab initio study. <i>Thermochimica Acta</i> , 2004, 418, 3-9.	1.2	54
66	The structural, electronic and vibrational properties of LiOH and NaOH: an ab initio study. <i>Chemical Physics Letters</i> , 2004, 387, 453-459.	1.2	54
67	Ab initio quantum mechanical study of γ -AlOOH boehmite: structure and vibrational spectrum. <i>Physics and Chemistry of Minerals</i> , 2009, 36, 47-59.	0.3	54
68	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
69	Seeds of Life in Space (SOLIS). <i>Astronomy and Astrophysics</i> , 2017, 605, A57.	2.1	54
70	Reactions of silica strained rings: an experimental and ab-initio study. <i>Surface Science</i> , 1995, 323, 151-162.	0.8	53
71	Vibrational Spectrum of Katoite Ca ₃ Al ₂ [(OH) ₄] ₃ : A Periodic ab Initio Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 692-701.	1.2	53
72	H-Chabazite with variable Si/Al ratio: stability and OH vibrational frequency computed in a periodic LCAO B3-LYP approach. <i>Chemical Physics Letters</i> , 2000, 318, 247-255.	1.2	52

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73	Large-Scale B3LYP Simulations of Ibuprofen Adsorbed in MCM-41 Mesoporous Silica as Drug Delivery System. <i>Journal of Physical Chemistry C</i> , 2014, 118, 26737-26749.	1.5	52
74	A Nanostructured Porous Silicon Near Insulator Becomes Either a p- or an n-Type Semiconductor upon Gas Adsorption. <i>Advanced Materials</i> , 2005, 17, 528-531.	11.1	51
75	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
76	Does Adsorption at Hydroxyapatite Surfaces Induce Peptide Folding? Insights from Large-Scale B3LYP Calculations. <i>Journal of the American Chemical Society</i> , 2012, 134, 10899-10910.	6.6	51
77	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
78	Ammonia and water as probes for the surface reactivity of covalent solids: cristobalite and silicon carbide. <i>Journal of the Chemical Society, Faraday Transactions</i> , 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. <i>Journal of Catalysis</i> , 2007, 245, 285-300.	3.1	50
80	Physico-Chemical Features of Aluminum Hydroxides As Modeled with the Hybrid B3LYP Functional and Localized Basis Functions. <i>Journal of Physical Chemistry C</i> , 2011, 115, 13107-13134.	1.5	50
81	Vibrational modes of isolated hydroxyls of silica computed ab initio in a cluster approach. <i>Chemical Physics Letters</i> , 1998, 294, 103-108.	1.2	49
82	CO/MgO(001) at different CO coverages: a periodic ab initio Hartree-Fock and B3-LYP study. <i>Surface Science</i> , 2001, 479, 255-272.	0.8	48
83	Coordination chemistry of Ca sites at the surface of nanosized hydroxyapatite: interaction with H ₂ O and CO. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2012, 370, 1313-1336.	1.6	48
84	Neutral vs Zwitterionic Glycine Forms at the Water/Silica Interface: Structure, Energies, and Vibrational Features from B3LYP Periodic Simulations. <i>Langmuir</i> , 2008, 24, 14027-14034.	1.6	47
85	Atomistic Model of Micelle-Templated Mesoporous Silicas: Structural, Morphological, and Adsorption Properties. <i>Langmuir</i> , 2012, 28, 11131-11141.	1.6	47
86	Silica-Based Materials as Drug Adsorbents: First Principle Investigation on the Role of Water Microsolvation on Ibuprofen Adsorption. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5801-5807.	1.1	47
87	Induced heterogeneity at the surface of group 4 dioxides as revealed by CO adsorption at room temperature. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1992, 88, 391.	1.7	45
88	A quantum mechanical study of the reactivity of (SiO) ₂ -defective silica surfaces. <i>Journal of Chemical Physics</i> , 2008, 128, 204702.	1.2	45
89	Hydrogarnet defect in chabazite and sodalite zeolites: A periodic Hartree-Fock and B3-LYP study. <i>Journal of Chemical Physics</i> , 2002, 117, 5337-5346.	1.2	44
90	Role of Mineral Surfaces in Prebiotic Chemical Evolution. In <i>Silico Quantum Mechanical Studies</i> . Life, 2019, 9, 10.	1.1	44

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91	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
92	Synthesis and Structural Investigation of Zr(BH ₄) ₄ . <i>Journal of Physical Chemistry C</i> , 2012, 116, 20239-20245.	1.5	43
93	A new massively parallel version of CRYSTAL for large systems on high performance computing architectures. <i>Journal of Computational Chemistry</i> , 2012, 33, 2276-2284.	1.5	43
94	B3LYP Simulation of the Full Vibrational Spectrum of 45S5 Bioactive Silicate Glass Compared to v-Silica. <i>Chemistry of Materials</i> , 2008, 20, 5610-5621.	3.2	42
95	Quantum Mechanical Investigations on the Formation of Complex Organic Molecules on Interstellar Ice Mantles. Review and Perspectives. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 1499-1523.	1.2	41
96	Experimental evidence for the hyperfine interaction between a surface superoxide species on MgO and a neighbouring hydroxylic proton. <i>Journal of the Chemical Society Faraday Transactions I</i> , 1989, 85, 3987.	1.0	40
97	Structure and Energetics of SiO ₂ Polymorphs by Quantum-Mechanical and Semiclassical Approaches. <i>Journal of Physical Chemistry B</i> , 2000, 104, 7259-7265.	1.2	40
98	Ab initio modeling of protein/biomaterial interactions: competitive adsorption between glycine and water onto hydroxyapatite surfaces. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 9005.	1.3	40
99	Vibrational Properties of MBH ₄ and MBF ₄ Crystals (M = Li, Na, K): A Combined DFT, Infrared, and Raman Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 18890-18900.	1.5	39
100	Toward a Surface Science Model for Biology: Glycine Adsorption on Nanohydroxyapatite with Well-Defined Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1390-1394.	2.1	38
101	Elastic and Vibrational Properties of $\hat{1}\pm$ - and $\hat{1}^2$ -PbO.. <i>Journal of Physical Chemistry C</i> , 2012, 116, 21514-21522.	1.5	38
102	The Surface of Ordered Mesoporous Benzene–Silica Hybrid Material: An Infrared and ab Initio Molecular Modeling Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 11961-11966.	1.2	36
103	A computational study on the effect of fluorine substitution in LiBH ₄ . <i>Journal of Alloys and Compounds</i> , 2011, 509, S679-S683.	2.8	36
104	Stability of the Dipolar (001) Surface of Hydroxyapatite. <i>Journal of Physical Chemistry C</i> , 2012, 116, 6108-6114.	1.5	36
105	Glycine Adsorption at Nonstoichiometric (010) Hydroxyapatite Surfaces: A B3LYP Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 14561-14567.	1.5	36
106	Chemical Desorption versus Energy Dissipation: Insights from Ab Initio Molecular Dynamics of HCO ⁺ Formation. <i>Astrophysical Journal</i> , 2020, 897, 56.	1.6	36
107	Density functional study of hydrogen-bonded systems: Energetic and vibrational features of some gas-phase adducts of hydrogen fluoride. <i>Computational and Theoretical Chemistry</i> , 1997, 419, 227-238.	1.5	35
108	Peptide bond formation activated by the interplay of Lewis and Brønsted catalysts. <i>Chemical Physics Letters</i> , 2005, 408, 295-301.	1.2	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. <i>American Mineralogist</i> , 2013, 98, 410-416.	0.9	35
110	DFT investigation of structural and vibrational properties of type B and mixed A-B carbonated hydroxylapatite. <i>American Mineralogist</i> , 2014, 99, 117-127.	0.9	35
111	Exfoliation Energy of Layered Materials by DFT-D: Beware of Dispersion!. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5244-5252.	2.3	35
112	Relative propensity of methanol and silanol towards hydrogen bond formation. <i>Chemical Physics Letters</i> , 1992, 191, 537-547.	1.2	34
113	Periodic B3LYP study of hydroxyapatite (001) surface modelled by thin layer slabs. <i>European Journal of Mineralogy</i> , 2007, 19, 757-767.	0.4	34
114	Theoretical Study of Molecular Hydrogen Adsorption in Mg-Exchanged Chabazite. <i>Journal of Physical Chemistry C</i> , 2007, 111, 1871-1873.	1.5	34
115	Functionalization of Zeolitic Cavities: Grafting NH ₂ Groups in Framework T Sites of B-SSZ-13 A Way to Obtain Basic Solids Catalysts?. <i>Journal of the American Chemical Society</i> , 2007, 129, 12131-12140.	6.6	34
116	MOLDRAW: Molecular graphics on a personal computer. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 1993, 208, 383-383.	0.4	33
117	Cage-like clusters as models for the hydroxyls of silica: ab initio calculation of ¹ H and ²⁹ Si NMR chemical shifts. <i>Chemical Physics Letters</i> , 1999, 299, 443-450.	1.2	33
118	Silanol as a model for the free hydroxyl of amorphous silica: comparison between experimental and calculated ab initio vibrational features. <i>Journal of Molecular Catalysis</i> , 1989, 54, 439-443.	1.2	32
119	Carbon monoxide adsorption on alkali and proton-exchanged chabazite: an ab-initio periodic study using the CRYSTAL code. <i>Molecular Physics</i> , 2005, 103, 2559-2571.	0.8	32
120	An ab initio parameterized interatomic force field for hydroxyapatite. <i>Journal of Materials Chemistry</i> , 2007, 17, 2061.	6.7	32
121	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
122	A computational multiscale strategy to the study of amorphous materials. <i>Theoretical Chemistry Accounts</i> , 2007, 117, 933-942.	0.5	32
123	Periodic B3-LYP calculations on H-Edingtonites, both alone and interacting with acetylene. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 545-553.	1.3	31
124	How Does Collagen Adsorb on Hydroxyapatite? Insights From Ab Initio Simulations on a Polyproline Type II Model. <i>Journal of Physical Chemistry C</i> , 2019, 123, 7540-7550.	1.5	31
125	Ab initio modelling of protein-biomaterial interactions: influence of amino acid polar side chains on adsorption at hydroxyapatite surfaces. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2012, 370, 1478-1498.	1.6	30
126	Theoretical and Experimental Study of LiBH ₄ -LiCl Solid Solution. <i>Crystals</i> , 2012, 2, 144-158.	1.0	30

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127	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
128	Stereospecific synthesis of squalenoid epoxide vinyl ethers as inhibitors of 2,3-oxidosqualene cyclase. <i>Journal of the Chemical Society Perkin Transactions 1</i> , 1988, , 461-469.	0.9	29
129	Infrared Spectroscopy Study of the Adsorption of Carbonyl Compounds on Severely Outgassed Silica: Spectroscopic and Thermodynamic Results. <i>Langmuir</i> , 1995, 11, 4811-4817.	1.6	29
130	VitaminC at 120K: experimental and theoretical study of the charge density. <i>Computational and Theoretical Chemistry</i> , 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. <i>Journal of Physical Chemistry C</i> , 2008, 112, 16879-16892.	1.5	29
132	Water at hydroxyapatite surfaces: the effect of coverage and surface termination as investigated by all-electron B3LYP-D* simulations. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	29
133	IR Study of the Adsorption of Unsaturated Hydrocarbons on Highly Outgassed Silica: Spectroscopic and Thermodynamic Results. <i>Langmuir</i> , 1997, 13, 5107-5113.	1.6	28
134	Molecular Water on Exposed Al ³⁺ Cations Is a Source of Acidity in Silicoaluminas. <i>Journal of Physical Chemistry B</i> , 2006, 110, 19087-19092.	1.2	28
135	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
136	Seeds of Life in Space (SOLIS). III. Zooming Into the Methanol Peak of the Prestellar Core L1544*. <i>Astrophysical Journal</i> , 2018, 855, 112.	1.6	28
137	Periodic DFT Study of Radical Species on Crystalline Silica Surfaces. <i>Journal of Physical Chemistry C</i> , 2010, 114, 16430-16438.	1.5	27
138	Affinity of hydroxyapatite (001) and (010) surfaces to formic and alendronic acids: a quantum-mechanical and infrared study. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 1099-1111.	1.3	27
139	Simulation and Experiment Reveal a Complex Scenario for the Adsorption of an Antifungal Drug in Ordered Mesoporous Silica. <i>Journal of Physical Chemistry C</i> , 2015, 119, 13068-13079.	1.5	27
140	Comparison of different approaches to the study of local defects in crystals. I. Theoretical considerations and computational schemes. <i>Physica Status Solidi (B): Basic Research</i> , 1983, 116, 249-259.	0.7	26
141	Ab initio study of the gas-phase equilibrium between (H ₂ O) ₄ and (H ₂ O) ₈ . <i>Chemical Physics Letters</i> , 1993, 212, 644-648.	1.2	26
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