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	Water Interaction with Fe2NiP Schreibersite (110) Surface: a Quantum Mechanical Atomistic Perspective. Journal of Physical Chemistry C, 2022, 126, 2243-2252.	3.1	1
2	From gaseous HCN to nucleobases at the cosmic silicate dust surface: an experimental insight into the onset of prebiotic chemistry in space. Physical Chemistry Chemical Physics, 2022, 24, 7224-7230.	2.8	3
3	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
4	Quantum Mechanical Simulations of the Radicalâ€"Radical Chemistry on Icy Surfaces. Astrophysical Journal, Supplement Series, 2022, 259, 39.	7.7	24
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.	2.7	19
6	Computer Generated Realistic Interstellar Icy Grain Models: Physicochemical Properties and Interaction with NH₃. ACS Earth and Space Chemistry, 2022, 6, 1286-1298.	2.7	11
7	Tracing the Primordial Chemical Life of Glycine: A Review from Quantum Chemical Simulations. International Journal of Molecular Sciences, 2022, 23, 4252.	4.1	12
8	Theoretical Distribution of the Ammonia Binding Energy at Interstellar Icy Grains: A New Computational Framework. ACS Earth and Space Chemistry, 2022, 6, 1514-1526.	2.7	18
9	Molecular recognition between membrane epitopes and nearly free surface silanols explains silica membranolytic activity. Colloids and Surfaces B: Biointerfaces, 2022, 217, 112625.	5.0	16
10	Ab initio Calculation of Binding Energies of Interstellar Sulphur-Containing Species on Crystalline Water Ice Models. Lecture Notes in Computer Science, 2021, , 608-619.	1.3	1
11	Computing Binding Energies of Interstellar Molecules by Semiempirical Quantum Methods: Comparison Between DFT and GFN2 on Crystalline Ice. Lecture Notes in Computer Science, 2021, , 632-645.	1.3	3
12	Balancing Cost and Accuracy in Quantum Mechanical Simulations on Collagen Protein Models. Journal of Chemical Theory and Computation, 2021, 17, 2566-2574.	5.3	9
13	Interaction of HCO+ Cations With Interstellar Negative Grains. Quantum Chemical Investigation and Astrophysical Implications. Frontiers in Astronomy and Space Sciences, 2021, 8, .	2.8	5
14	Ab Initio Computational Study on Fe2NiP Schreibersite: Bulk and Surface Characterization. ACS Earth and Space Chemistry, 2021, 5, 1741-1751.	2.7	6
15	Theoretical computations on the efficiency of acetaldehyde formation on interstellar icy grains. Astronomy and Astrophysics, 2021, 655, A9.	5.1	18
16	H₂ Formation on Interstellar Grains and the Fate of Reaction Energy. Astrophysical Journal, 2021, 917, 49.	4.5	26
17	Infrared harmonic features of collagen models at B3LYP-D3: From amide bands to the THz region. Journal of Chemical Physics, 2021, 155, 075102.	3.0	5
18	Structures and Properties of Known and Postulated Interstellar Cations. Astrophysical Journal, Supplement Series, 2021, 256, 35.	7.7	4

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19	Computational Surface Modelling of Ices and Minerals of Interstellar Interestâ€"Insights and Perspectives. Minerals (Basel, Switzerland), 2021, 11, 26.	2.0	13
20	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.	5.4	2
21	The rise of computer modeling in prebiotic chemistry. Physics of Life Reviews, 2020, 34-35, 139-142.	2.8	4
22	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
23	Monitoring the Reactivity of Formamide on Amorphous SiO2 by In-Situ UV-Raman Spectroscopy and DFT Modeling. Molecules, 2020, 25, 2274.	3.8	3
24	A quantum mechanical study of dehydrationvs.decarbonylation of formamide catalysed by amorphous silica surfaces. Physical Chemistry Chemical Physics, 2020, 22, 8353-8363.	2.8	7
25	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
26	Exfoliation Energy of Layered Materials by DFT-D: Beware of Dispersion!. Journal of Chemical Theory and Computation, 2020, 16, 5244-5252.	5.3	35
27	Chemical Desorption versus Energy Dissipation: Insights from Ab Initio Molecular Dynamics of HCOÂ· Formation. Astrophysical Journal, 2020, 897, 56.	4.5	36
28	On the Surface Acidâ€"Base Properties of Amorphous and Crystalline Mg₂SiO₄ as Probed by Adsorbed CO, CO₂, and CD₃CN. ACS Earth and Space Chemistry, 2020, 4, 345-354.	2.7	5
29	Modeling Interstellar Amorphous Solid Water Grains by Tight-Binding Based Methods: Comparison Between GFN-XTB and CCSD(T) Results for Water Clusters. Lecture Notes in Computer Science, 2020, , 745-753.	1.3	4
30	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
31	Formamide Dehydration and Condensation on Acidic Montmorillonite: Mechanistic Insights from Ab-Initio Periodic Simulations. Lecture Notes in Computer Science, 2020, , 502-512.	1.3	0
32	Decoding Collagen Triple Helix Stability by Means of Hybrid DFT Simulations. Journal of Physical Chemistry B, 2019, 123, 7354-7364.	2.6	14
33	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
34	What Can Infrared Spectra Tell Us about the Crystallinity of Nanosized Interstellar Silicate Dust Grains?. ACS Earth and Space Chemistry, 2019, 3, 2323-2338.	2.7	18
35	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
36	Cost-Effective Quantum Mechanical Approach for Predicting Thermodynamic and Mechanical Stability of Pure-Silica Zeolites. ACS Omega, 2019, 4, 1838-1846.	3.5	17

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37	Role of Mineral Surfaces in Prebiotic Chemical Evolution. In Silico Quantum Mechanical Studies. Life, 2019, 9, 10.	2.4	44
38	Carbon monoxide adsorption at forsterite surfaces as models of interstellar dust grains: An unexpected bathochromic (red) shift of the CO stretching frequency. Journal of Chemical Physics, 2019, 150, 064702.	3.0	4
39	Elucidating the Nature of Interactions in Collagen Triple-Helix Wrapping. Journal of Physical Chemistry Letters, 2019, 10, 7644-7649.	4.6	10
40	Silicate-mediated interstellar water formation: a theoretical study. Monthly Notices of the Royal Astronomical Society, 2019, 482, 5389-5400.	4.4	22
41	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
42	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
43	Properties and Reactivity toward Water of A Type Carbonated Apatite and Hydroxyapatite Surfaces. Journal of Physical Chemistry C, 2018, 122, 3934-3944.	3.1	18
44	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
45	Working at the membrane interface: Ligandâ€induced changes in dynamic conformation and oligomeric structure in human aromatase. Biotechnology and Applied Biochemistry, 2018, 65, 46-53.	3.1	16
46	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, .	3.3	0
47	Formamide Adsorption at the Amorphous Silica Surface: A Combined Experimental and Computational Approach. Life, 2018, 8, 42.	2.4	14
48	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.	3.3	23
49	Ab Initio Modeling of Hydrogen Bond Interaction at Silica Surfaces With Focus on Silica/Drugs Systems. , 2018, , 297-328.		6
50	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
51	Can Formamide Be Formed on Interstellar Ice? An Atomistic Perspective. ACS Earth and Space Chemistry, 2018, 2, 720-734.	2.7	83
52	Models for biomedical interfaces: a computational study of quinone-functionalized amorphous silica surface features. Physical Chemistry Chemical Physics, 2017, 19, 7793-7806.	2.8	11
53	Topical collection of papers collected on the occasion of the XLI congress of the theoretical chemists of Latin expression (CHITEL 2015 - Torino - Italy). Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	0
54	Method Dependence of Proline Ring Flexibility in the Poly-<scp>l</scp>-Proline Type II Polymer. Journal of Chemical Theory and Computation, 2017, 13, 370-379.	5.3	16

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55	Modeling hydroxylated nanosilica: Testing the performance of ReaxFF and FFSiOH force fields. Journal of Chemical Physics, 2017, 146, 224704.	3.0	12
56	How strong are H-bonds at the fully hydroxylated silica surfaces? Insights from the B3LYP electron density topological analysis. Structural Chemistry, 2017, 28, 1009-1015.	2.0	15
57	Seeds of Life in Space (SOLIS). Astronomy and Astrophysics, 2017, 605, A57.	5.1	54
58	Forsterite Surfaces as Models of Interstellar Core Dust Grains: Computational Study of Carbon Monoxide Adsorption. ACS Earth and Space Chemistry, 2017, 1, 384-398.	2.7	21
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.	4.5	116
60	Computing Free Energies of Hydroxylated Silica Nanoclusters: Forcefield versus Density Functional Calculations. Inorganics, 2017, 5, 41.	2.7	3
61	Seeds of Life in Space (SOLIS). Astronomy and Astrophysics, 2017, 605, L3.	5.1	98
62	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.	4.1	22
63	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
64	Propionic acid derivatives confined in mesoporous silica: monomers or dimers? The case of ibuprofen investigated by static and dynamic ab initio simulations. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	6
65	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
66	Elucidating the fundamental forces in protein crystal formation: the case of crambin. Chemical Science, 2016, 7, 1496-1507.	7.4	21
67	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
68	Surface Modeling of Ceramic Biomaterials. , 2016, , 3935-3947.		0
69	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
70	Strained ring motif at silica surfaces: A quantum mechanical study of their reactivity towards protic molecules. Computational and Theoretical Chemistry, 2015, 1074, 168-177.	2.5	10
71	Computational Study of Acidic and Basic Functionalized Crystalline Silica Surfaces as a Model for Biomaterial Interfaces. Langmuir, 2015, 31, 6321-6331.	3.5	11
72	Electronic Structure of Ti³⁺â€“Ethylene Complexes in Microporous Aluminophosphate Materials. A Combined EPR and DFT Study Elucidating the Role of SOMO Orbitals in Metalâ€“Olefin Ï€ Complexes. Journal of Physical Chemistry C, 2015, 119, 26046-26055.	3.1	6

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73	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
74	Surface Modeling of Ceramic Biomaterials. , 2015, , 1-13.		0
75	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
76	CO₃^{2â€“} Mobility in Carbonate Apatite As Revealed by Density Functional Modeling. Journal of Physical Chemistry C, 2014, 118, 1364-1369.	3.1	20
77	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
78	Halide substitution in Ca(BH₄)₂. RSC Advances, 2014, 4, 4736-4742.	3.6	22
79	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
80	Probing the fate of interstitial water in bulk bioactive glass by ab initio simulations. RSC Advances, 2014, 4, 36425-36436.	3.6	14
81	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
82	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.	2.5	20
83	Effects of metastability on hydrogen sorption in fluorine substituted hydrides. Journal of Alloys and Compounds, 2014, 615, S706-S710.	5.5	12
84	Combined quantum chemical and modeling study of CO hydrogenation on water ice. Astronomy and Astrophysics, 2014, 572, A70.	5.1	87
85	Revealing Hydroxyapatite Nanoparticle Surface Structure by CO Adsorption: A Combined B3LYP and Infrared Study. Journal of Physical Chemistry C, 2013, 117, 25526-25534.	3.1	18
86	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
87	Silica Surface Features and Their Role in the Adsorption of Biomolecules: Computational Modeling and Experiments. Chemical Reviews, 2013, 113, 4216-4313.	47.7	508
88	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
89	The vibrational features of hydroxylapatite and type A carbonated apatite: A first principle contribution. American Mineralogist, 2013, 98, 752-759.	1.9	55
90	DFT Modeling of 45S5 and 77S Soda-Lime Phospho-Silicate Glass Surfaces: Clues on Different Bioactivity Mechanism. Langmuir, 2013, 29, 5749-5759.	3.5	20

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91	Thermodynamic Tuning of Calcium Hydride by Fluorine Substitution. Materials Research Society Symposia Proceedings, 2012, 1441, 17.	0.1	6
92	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
93	COMPUTATIONAL STUDY OF INTERSTELLAR GLYCINE FORMATION OCCURRING AT RADICAL SURFACES OF WATER-ICE DUST PARTICLES. Astrophysical Journal, 2012, 754, 24.	4.5	51
94	Elastic and Vibrational Properties of Î±- and Î²-PbO.. Journal of Physical Chemistry C, 2012, 116, 21514-21522.	3.1	38
95	Stability of the Dipolar (001) Surface of Hydroxyapatite. Journal of Physical Chemistry C, 2012, 116, 6108-6114.	3.1	36
96	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
97	Computational Simulations of Prebiotic Processes. Cellular Origin and Life in Extreme Habitats, 2012, , 345-362.	0.3	1
98	Glycine Adsorption at Nonstoichiometric (010) Hydroxyapatite Surfaces: A B3LYP Study. Journal of Physical Chemistry C, 2012, 116, 14561-14567.	3.1	36
99	Synthesis and Structural Investigation of Zr(BH₄)₄. Journal of Physical Chemistry C, 2012, 116, 20239-20245.	3.1	43
100	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
101	Prebiotic chemistry. Chemical Society Reviews, 2012, 41, 5373.	38.1	13
102	Atomistic Model of Micelle-Templated Mesoporous Silicas: Structural, Morphological, and Adsorption Properties. Langmuir, 2012, 28, 11131-11141.	3.5	47
103	Theoretical and Experimental Study of LiBH4-LiCl Solid Solution. Crystals, 2012, 2, 144-158.	2.2	30
104	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
105	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
106	Silanol-Related and Unspecific Adsorption of Molecular Ammonia on Highly Dehydrated Silica. Journal of Physical Chemistry C, 2011, 115, 23344-23353.	3.1	19
107	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
108	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

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109	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
110	Experimental and computational investigations on the AlH3/AlF3 system. Journal of Alloys and Compounds, 2011, 509, 10-14.	5.5	19
111	A computational study on the effect of fluorine substitution in LiBH4. Journal of Alloys and Compounds, 2011, 509, S679-S683.	5.5	36
112	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
113	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
114	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
115	In silico study of the interstellar prebiotic formation and delivery of glycine. Rendiconti Lincei, 2011, 22, 137-144.	2.2	10
116	J-ICE: a newJmolinterface for handling and visualizing crystallographic and electronic properties. Journal of Applied Crystallography, 2011, 44, 225-229.	4.5	88
117	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
118	Probing vibrational modes in silica glass using inelastic neutron scattering with mass contrast. Physical Review B, 2010, 81, .	3.2	14
119	Crystal structure of thioflavin-T and its binding to amyloid fibrils: insights at the molecular level. Chemical Communications, 2010, 46, 1156.	4.1	78
120	Hydrophobic Behavior of Dehydroxylated Silica Surfaces: A B3LYP Periodic Study. Journal of Physical Chemistry C, 2010, 114, 19984-19992.	3.1	23
121	Search and Characterization of Transition State Structures in Crystalline Systems Using Valence Coordinates. Journal of Chemical Theory and Computation, 2010, 6, 1341-1350.	5.3	19
122	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
123	Thermodynamic Database for Hydrogen Storage Materials. Advances in Science and Technology, 2010, 72, 213-218.	0.2	11
124	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
125	Periodic DFT Study of Radical Species on Crystalline Silica Surfaces. Journal of Physical Chemistry C, 2010, 114, 16430-16438.	3.1	27
126	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

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127	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
128	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
129	Ab initio modeling of layered materials with the CRYSTAL code: an overview. Zeitschrift FÃ¼r Kristallographie, 2009, 224, 241-250.	1.1	8
130	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
131	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
132	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
133	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
134	Water Adsorption on the Stoichiometric (001) and (010) Surfaces of Hydroxyapatite: A Periodic B3LYP Study. Langmuir, 2009, 25, 2188-2198.	3.5	80
135	Affinity Scale for the Interaction of Amino Acids with Silica Surfaces. Journal of Physical Chemistry C, 2009, 113, 5741-5750.	3.1	105
136	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
137	The role of defective silica surfaces in exogenous delivery of prebiotic compounds: clues from first principles calculations. Physical Chemistry Chemical Physics, 2009, 11, 2497.	2.8	21
138	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
139	A review of the computational studies of proton- and metal-exchanged chabazites as media for molecular hydrogen storage performed with the CRYSTAL code. International Journal of Hydrogen Energy, 2008, 33, 746-754.	7.1	20
140	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
141	Testing the combination of Hartreeâ€“Fock exchange and Wilsonâ€“Levy correlation for weakly bonded extended systems. Chemical Physics Letters, 2008, 451, 287-292.	2.6	15
142	Hydroxylated crystalline edingtonite silica faces as models for the amorphous silica surface. Journal of Physics: Conference Series, 2008, 117, 012026.	0.4	13
143	B3LYP augmented with an empirical dispersion term (B3LYP-D*) as applied to molecular crystals. CrystEngComm, 2008, 10, 405-410.	2.6	775
144	IR and Computational Characterization of CO Adsorption on a Model Surface, the Phenylene Periodic Mesoporous Organosilca with Crystalline Walls. Journal of Physical Chemistry C, 2008, 112, 19560-19567.	3.1	18

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145	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
146	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
147	A quantum mechanical study of the reactivity of (SiO)2-defective silica surfaces. Journal of Chemical Physics, 2008, 128, 204702.	3.0	45
148	B3LYP Simulation of the Full Vibrational Spectrum of 45S5 Bioactive Silicate Glass Compared to v-Silica. Chemistry of Materials, 2008, 20, 5610-5621.	6.7	42
149	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
150	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
151	Ab Initioinvestigation of the interaction of H₂with lithium exchanged low-silica chabazites. Journal of Physics: Conference Series, 2008, 117, 012012.	0.4	3
152	Periodic B3LYP study of hydroxyapatite (001) surface modelled by thin layer slabs. European Journal of Mineralogy, 2007, 19, 757-767.	1.3	34
153	An ab initio parameterized interatomic force field for hydroxyapatite. Journal of Materials Chemistry, 2007, 17, 2061.	6.7	32
154	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
155	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
156	Theoretical Study of Molecular Hydrogen Adsorption in Mg-Exchanged Chabazite. Journal of Physical Chemistry C, 2007, 111, 1871-1873.	3.1	34
157	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
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