

Xiancai Lu

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

159
papers

2,689
citations

30
h-index

43
g-index

162
ext. papers

3,226
ext. citations

4.5
avg, IF

5.3
L-index

#	Paper	IF	Citations
159	Acidity of edge surface sites of montmorillonite and kaolinite. <i>Geochimica Et Cosmochimica Acta</i> , 2013 , 117, 180-190	5.5	146
158	A thermodynamic understanding of clay-swelling inhibition by potassium ions. <i>Angewandte Chemie - International Edition</i> , 2006 , 45, 6300-3	16.4	104
157	Surface Wettability of Basal Surfaces of Clay Minerals: Insights from Molecular Dynamics Simulation. <i>Energy & Fuels</i> , 2016 , 30, 149-160	4.1	70
156	Source rocks in Mesozoic-Cenozoic continental rift basins, east China: A case from Dongying Depression, Bohai Bay Basin. <i>Organic Geochemistry</i> , 2009 , 40, 229-242	3.1	70
155	Deformation of Coal Induced by Methane Adsorption at Geological Conditions. <i>Energy & Fuels</i> , 2010 , 24, 5955-5964	4.1	69
154	Surface acidity of 2:1-type dioctahedral clay minerals from first principles molecular dynamics simulations. <i>Geochimica Et Cosmochimica Acta</i> , 2014 , 140, 410-417	5.5	63
153	Hydration and Mobility of Interlayer Ions of (Na _x , Ca _y)-Montmorillonite: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 29811-29821	3.8	63
152	Effects of layer-charge distribution on the thermodynamic and microscopic properties of Cs-smectite. <i>Geochimica Et Cosmochimica Acta</i> , 2008 , 72, 1837-1847	5.5	61
151	Nanogeosciences: Research History, Current Status, and Development Trends. <i>Journal of Nanoscience and Nanotechnology</i> , 2017 , 17, 5930-5965	1.3	60
150	Interlayer structure and dynamics of alkylammonium-intercalated smectites with and without water: A molecular dynamics study. <i>Clays and Clay Minerals</i> , 2007 , 55, 554-564	2.1	58
149	Microbial Oxidation of Sulfide Tailings and the Environmental Consequences. <i>Elements</i> , 2012 , 8, 119-124	3.8	54
148	Atomic-scale structures of interfaces between phyllosilicate edges and water. <i>Geochimica Et Cosmochimica Acta</i> , 2012 , 81, 56-68	5.5	54
147	Quantitative X-ray photoelectron spectroscopy-based depth profiling of bioleached arsenopyrite surface by <i>Acidithiobacillus ferrooxidans</i> . <i>Geochimica Et Cosmochimica Acta</i> , 2014 , 127, 120-139	5.5	49
146	Hydration of methane intercalated in Na-smectites with distinct layer charge: insights from molecular simulations. <i>Journal of Colloid and Interface Science</i> , 2011 , 355, 237-42	9.3	47
145	Understanding surface acidity of gibbsite with first principles molecular dynamics simulations. <i>Geochimica Et Cosmochimica Acta</i> , 2013 , 120, 487-495	5.5	46
144	Molecular dynamics insight into the cointercalation of hexadecyltrimethyl-ammonium and acetate ions into smectites. <i>American Mineralogist</i> , 2009 , 94, 143-150	2.9	46
143	Surface complexation of heavy metal cations on clay edges: insights from first principles molecular dynamics simulation of Ni(II). <i>Geochimica Et Cosmochimica Acta</i> , 2017 , 203, 54-68	5.5	41

142	Structural Incorporation of Manganese into Goethite and Its Enhancement of Pb(II) Adsorption. <i>Environmental Science & Technology</i> , 2018 , 52, 4719-4727	10.3	40
141	Hydration mechanisms of Cu(2+): tetra-, penta- or hexa-coordinated?. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 10801-4	3.6	39
140	Atomic scale structures of interfaces between kaolinite edges and water. <i>Geochimica Et Cosmochimica Acta</i> , 2012 , 92, 233-242	5.5	38
139	Reduction of jarosite by <i>Shewanella oneidensis</i> MR-1 and secondary mineralization. <i>Geochimica Et Cosmochimica Acta</i> , 2014 , 124, 54-71	5.5	37
138	Occurrence of stable and mobile organic matter in the clay-sized fraction of shale: Significance for petroleum geology and carbon cycle. <i>International Journal of Coal Geology</i> , 2016 , 160-161, 1-10	5.5	36
137	Surface acidity of quartz: understanding the crystallographic control. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 26909-16	3.6	35
136	Speciation of gold in hydrosulphide-rich ore-forming fluids: Insights from first-principles molecular dynamics simulations. <i>Geochimica Et Cosmochimica Acta</i> , 2011 , 75, 185-194	5.5	35
135	Acid dissociation mechanisms of Si(OH) ₄ and Al(H ₂ O) ₆ ³⁺ in aqueous solution. <i>Geochimica Et Cosmochimica Acta</i> , 2010 , 74, 510-516	5.5	35
134	Effects of CO ₂ adsorption on coal deformation during geological sequestration. <i>Journal of Geophysical Research</i> , 2011 , 116,		34
133	Sorption and desorption of phenanthrene onto iron, copper, and silicon dioxide nanoparticles. <i>Langmuir</i> , 2008 , 24, 10929-35	4	34
132	Solution Structures and Acidity Constants of Molybdic Acid. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 2926-2930	6.4	33
131	Mountain biodiversity and ecosystem functions: interplay between geology and contemporary environments. <i>ISME Journal</i> , 2020 , 14, 931-944	11.9	33
130	Secondary minerals of weathered orpiment-realgar-bearing tailings in Shimen carbonate-type realgar mine, Changde, Central China. <i>Mineralogy and Petrology</i> , 2015 , 109, 1-15	1.6	31
129	Silver speciation in chloride-containing hydrothermal solutions from first principles molecular dynamics simulations. <i>Chemical Geology</i> , 2012 , 294-295, 103-112	4.2	30
128	Surface complexes of acetate on edge surfaces of 2:1 type phyllosilicate: Insights from density functional theory calculation. <i>Geochimica Et Cosmochimica Acta</i> , 2008 , 72, 5896-5907	5.5	30
127	Cadmium(II) Complexes Adsorbed on Clay Edge Surfaces: Insight from First Principles Molecular Dynamics Simulation. <i>Clays and Clay Minerals</i> , 2016 , 64, 337-347	2.1	27
126	Porphyry and skarn Au-U deposits in the Shizishan orefield, Tongling, East China: U-Bb dating and in-situ Hf isotope analysis of zircons and petrogenesis of associated granitoids. <i>Ore Geology Reviews</i> , 2011 , 43, 182-193	3.2	26
125	Facet-Dependent Photodegradation of Methylene Blue by Hematite Nanoplates in Visible Light. <i>Environmental Science & Technology</i> , 2021 , 55, 677-688	10.3	26

124	Interfacial structures and acidity of edge surfaces of ferruginous smectites. <i>Geochimica Et Cosmochimica Acta</i> , 2015 , 168, 293-301	5.5	25
123	Collaborative effects of <i>Acidithiobacillus ferrooxidans</i> and ferrous ions on the oxidation of chalcopyrite. <i>Chemical Geology</i> , 2018 , 493, 109-120	4.2	24
122	Acidities of confined water in interlayer space of clay minerals. <i>Geochimica Et Cosmochimica Acta</i> , 2011 , 75, 4978-4986	5.5	22
121	Solvation forces between molecularly rough surfaces. <i>Journal of Colloid and Interface Science</i> , 2011 , 362, 382-8	9.3	21
120	Mediation of Extracellular Polymeric Substances in Microbial Reduction of Hematite by MR-1. <i>Frontiers in Microbiology</i> , 2019 , 10, 575	5.7	20
119	Temperature dependence of interfacial structures and acidity of clay edge surfaces. <i>Geochimica Et Cosmochimica Acta</i> , 2015 , 160, 91-99	5.5	20
118	Understanding hydration of Zn ²⁺ in hydrothermal fluids with ab initio molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 13305-9	3.6	20
117	Temperature-dependent phase transition and desorption free energy of sodium dodecyl sulfate at the water/vapor interface: approaches from molecular dynamics simulations. <i>Langmuir</i> , 2014 , 30, 10600-4	4	19
116	Bioleaching of chalcopyrite by <i>Acidithiobacillus ferrooxidans</i> . <i>Minerals Engineering</i> , 2013 , 53, 184-192	4.9	19
115	Petrogenesis of the Bao'an zhai granite and associated Mo mineralization, western Dabie orogen, east-central China: Constraints from zircon U-Pb and molybdenite Re-Os dating, whole-rock geochemistry, and Sr-Nd-Ba isotopes. <i>International Geology Review</i> , 2013 , 55, 1220-1238	2.3	19
114	Writable and Self-Erasable Hydrogel Based on Dissipative Assembly Process from Multiple Carboxyl Tetraphenylethylene Derivative 2020 , 2, 425-429		18
113	Interlayer Structure and Dynamics of HDTMA ⁺ -Intercalated Hectorite with and without Water: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 13071-13078	3.8	18
112	Influence of the temperature dependence of thermal parameters of heat conduction models on the reconstruction of thermal history of igneous-intrusion-bearing basins. <i>Computers and Geosciences</i> , 2010 , 36, 1339-1344	4.5	18
111	Sulfur Transformation in Microbially Mediated Pyrite Oxidation by <i>Acidithiobacillus ferrooxidans</i> : Insights From X-ray Photoelectron Spectroscopy-Based Quantitative Depth Profiling. <i>Geomicrobiology Journal</i> , 2016 , 33, 118-134	2.5	17
110	Comment on Influence of a basic intrusion on the vitrinite reflectance and chemistry of the Springfield (No. 5) coal, Harrisburg, Illinois by Stewart et al. (2005). <i>International Journal of Coal Geology</i> , 2008 , 73, 196-199	5.5	17
109	Numerical modelling of the hydrocarbon generation of Tertiary source rocks intruded by doleritic sills in the Zhanhua depression, Bohai Bay Basin, China. <i>Basin Research</i> , 2012 , 24, 234-247	3.2	16
108	Molecular simulation study on K ⁺ -Cl ⁻ ion pair in geological fluids. <i>Acta Geochimica</i> , 2017 , 36, 1-8	2.2	15
107	Helium diffusion in olivine based on first principles calculations. <i>Geochimica Et Cosmochimica Acta</i> , 2015 , 156, 145-153	5.5	15

106	Molecular Dynamics Simulation of the Effects of NaCl on Electrostatic Properties of Newton Black Films. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 21913-21922	3.8	15
105	Constraints on timing and origin of the Dayinjian intrusion and associated molybdenum mineralization, western Dabie orogen, central China. <i>International Geology Review</i> , 2012 , 54, 1579-1596	2.3	15
104	Mineralogical characteristics of unusual black talc ores in Guangfeng County, Jiangxi Province, China. <i>Applied Clay Science</i> , 2013 , 74, 37-46	5.2	15
103	Recent progress in studies on the nano-sized particle layer in rock shear planes. <i>Progress in Natural Science: Materials International</i> , 2008 , 18, 367-373	3.6	15
102	Heat-model analysis of wall rocks below a diabase sill in Huimin Sag, China compared with thermal alteration of mudstone to carbargilite and hornfels and with increase of vitrinite reflectance. <i>Geophysical Research Letters</i> , 2007 , 34,	4.9	15
101	Jumping Diffusion of Water Intercalated in Layered Double Hydroxides. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 12924-12931	3.8	14
100	In silico calculation of acidity constants of carbonic acid conformers. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 12914-7	2.8	14
99	Tolerance and Biosorption of Heavy Metals by <i>Cupriavidus metallidurans</i> strain XXKD-1 Isolated from a Subsurface Laneway in the Qixiashan Pb-Zn Sulfide Minery in Eastern China. <i>Geomicrobiology Journal</i> , 2012 , 29, 274-286	2.5	14
98	A combined first principles and classical molecular dynamics study of clay-soil organic matters (SOMs) interactions. <i>Geochimica Et Cosmochimica Acta</i> , 2020 , 291, 110-125	5.5	14
97	Coupling between clay swelling/collapse and cationic partition. <i>Geochimica Et Cosmochimica Acta</i> , 2020 , 285, 78-99	5.5	14
96	Synthesis of 2D Hexagonal Hematite Nanosheets and the Crystal Growth Mechanism. <i>Inorganic Chemistry</i> , 2019 , 58, 16727-16735	5.1	14
95	Structures and acidity constants of arsenite and thioarsenite species in hydrothermal solutions. <i>Chemical Geology</i> , 2015 , 411, 192-199	4.2	13
94	Complexation of heavy metal cations on clay edges at elevated temperatures. <i>Chemical Geology</i> , 2018 , 479, 36-46	4.2	13
93	Influences of Cation Ratio, Anion Type, and Water Content on Polytypism of Layered Double Hydroxides. <i>Inorganic Chemistry</i> , 2018 , 57, 7299-7313	5.1	13
92	Specific Counterion Effects on the Atomistic Structure and Capillary-Waves Fluctuation of the Water/Vapor Interface Covered by Sodium Dodecyl Sulfate. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 19205-19213	3.8	13
91	A rapid glacier surge on Mount Tobe Feng, western China, 2015. <i>Journal of Glaciology</i> , 2016 , 62, 407-409	3.4	12
90	Molecular simulation study of hydrated Na-rectorite. <i>Langmuir</i> , 2015 , 31, 2008-13	4	12
89	Ab Initio Molecular Dynamics Study of Fe-Containing Smectites. <i>Clays and Clay Minerals</i> , 2010 , 58, 89-96	2.1	12

88	Metallogenetic Mechanism and Timing of Late Superimposing Fluid Mineralization in the Dongguashan Diplogenetic Stratified Copper Deposit, Anhui Province. <i>Acta Geologica Sinica</i> , 2005 , 79, 405-413	0.7	12
87	Complexation of carboxylate on smectite surfaces. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 18400-18406	3.8	11
86	Regulates Biofilm Development of MnB1 as a Primary Response to HO and Mn. <i>Frontiers in Microbiology</i> , 2018 , 9, 1490	5.7	11
85	A new integrated method for characterizing surface energy heterogeneity from a single adsorption isotherm. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 15828-34	3.4	11
84	Slow dynamics of water confined in Newton black films. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 19183-93	3.6	10
83	Confined water in tunnel nanopores of sepiolite: Insights from molecular simulations. <i>American Mineralogist</i> , 2016 , 101, 713-718	2.9	10
82	The surface fractal investigation on carbon nanotubes modified by the adsorption of poly(acrylic acid). <i>Surface and Coatings Technology</i> , 2005 , 190, 394-399	4.4	10
81	New evidence of microbe origin for ferromanganese nodules from the East Pacific deep sea floor. <i>Science in China Series D: Earth Sciences</i> , 2000 , 43, 187-192		10
80	Acidity constants and redox potentials of uranyl ions in hydrothermal solutions. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 26040-26048	3.6	10
79	Selection of Planar Chiral Conformations between Pillar[5,6]arenes Induced by Amino Acid Derivatives in Aqueous Media. <i>Chemistry - A European Journal</i> , 2021 , 27, 5890-5896	4.8	10
78	First-principles molecular dynamics study of stepwise hydrolysis reactions of Y ³⁺ cations. <i>Chemical Geology</i> , 2012 , 334, 37-43	4.2	9
77	First-Principles Molecular Dynamics Insight into Fe ²⁺ Complexes Adsorbed on Edge Surfaces of Clay Minerals. <i>Clays and Clay Minerals</i> , 2012 , 60, 341-347	2.1	9
76	Tourmalines from the Koktokay No.3 pegmatite, Altai, NW China: spectroscopic characterization and relationships with the pegmatite evolution. <i>European Journal of Mineralogy</i> , 2008 , 20, 143-154	2.2	9
75	Discovery of low-mature hydrocarbon in manganese nodules and ooze from the Central Pacific deep sea floor. <i>Science Bulletin</i> , 2002 , 47, 939		9
74	Specificity of low molecular weight organic acids on the release of elements from lizardite during fungal weathering. <i>Geochimica Et Cosmochimica Acta</i> , 2019 , 256, 20-34	5.5	9
73	Understanding the Heterogeneous Nucleation of Heavy Metal Phyllosilicates on Clay Edges with First-Principles Molecular Dynamics. <i>Environmental Science & Technology</i> , 2019 , 53, 13704-13712	10.3	8
72	Analysis of Genes and Proteins in <i>Acidithiobacillus ferrooxidans</i> During Growth and Attachment on Pyrite Under Different Conditions. <i>Geomicrobiology Journal</i> , 2013 , 30, 255-267	2.5	8
71	Development of online instructional resources for Earth system science education: An example of current practice from China. <i>Computers and Geosciences</i> , 2009 , 35, 1271-1279	4.5	8

70	An atomic-scale understanding of the initial stage of nucleation of heavy metal cations on clay edges. <i>Geochimica Et Cosmochimica Acta</i> , 2019 , 248, 161-171	5.5	8
69	Geochemical fates and unusual distribution of arsenic in natural ferromanganese duricrust. <i>Applied Geochemistry</i> , 2017 , 76, 74-87	3.5	7
68	Molecular Dynamics Simulation of Alkylammonium-Intercalated Vermiculites. <i>Clays and Clay Minerals</i> , 2017 , 65, 378-386	2.1	7
67	Distribution and Mobility of Crude Oil-Brine in Clay Mesopores: Insights from Molecular Dynamics Simulations. <i>Langmuir</i> , 2019 , 35, 14818-14832	4	7
66	Oxidation and Mineralization of Mn ²⁺ Ions Mediated by <i>Pseudomonas putida</i> : Insights from an Experimental Study. <i>Acta Geologica Sinica</i> , 2017 , 91, 1276-1285	0.7	7
65	A comparative study of natural and experimental nano-sized grinding grain textures in rocks. <i>Science Bulletin</i> , 2008 , 53, 1217-1221	10.6	7
64	Thermodynamic properties in the Fe(II)-Fe(III)-As(V)-HClO ₄ -H ₂ O and Fe(II)-Fe(III)-As(V)-HCl-H ₂ O systems from 5 to 90 °C. <i>Chemical Geology</i> , 2017 , 460, 37-45	4.2	6
63	Superionic Silica-Water and Silica-Hydrogen Compounds in the Deep Interiors of Uranus and Neptune.. <i>Physical Review Letters</i> , 2022 , 128, 035702	7.4	6
62	Changes in the Interlayer Structure and Thermodynamics of Hydrated Montmorillonite Under Basin Conditions: Molecular Simulation Approaches. <i>Clays and Clay Minerals</i> , 2016 , 64, 503-511	2.1	6
61	Structures and Acidity Constants of Silver-Sulfide Complexes in Hydrothermal Fluids: A First-Principles Molecular Dynamics Study. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 8435-8443	2.8	6
60	On the thermodynamics and kinetics of scorodite dissolution. <i>Geochimica Et Cosmochimica Acta</i> , 2019 , 265, 468-477	5.5	5
59	First-Principles Study of Thermodynamics and Spin Transition in FeSiO ₃ Liquid at High Pressure. <i>Geophysical Research Letters</i> , 2019 , 46, 3706-3716	4.9	5
58	Microbial reductive transformation of iron-rich tailings in a column reactor and its environmental implications to arsenic reactive transport in mining tailings. <i>Science of the Total Environment</i> , 2019 , 670, 1008-1018	10.2	5
57	Interlayer Structures and Dynamics of Arsenate and Arsenite Intercalated Layered Double Hydroxides: A First Principles Study. <i>Minerals (Basel, Switzerland)</i> , 2017 , 7, 53	2.4	5
56	Atomistic simulation on mixing thermodynamics of calcite-smithsonite solid solutions. <i>American Mineralogist</i> , 2015 , 100, 172-180	2.9	5
55	Anorthite dissolution promoted by bacterial adhesion: Direct evidence from dialytic experiment. <i>Science China Earth Sciences</i> , 2011 , 54, 204-211	4.6	5
54	Roles of adhered <i>Paenibacillus polymyxa</i> in the dissolution and flotation of bauxite: a dialytic investigation. <i>Frontiers of Earth Science</i> , 2010 , 4, 167-173		5
53	Observation of ultra-microtexture of fault rocks in shearing-sliding zones*. <i>Progress in Natural Science: Materials International</i> , 2005 , 15, 430-434	3.6	5

52	A molecular dynamics simulation study of KF and NaF ion pairs in hydrothermal fluids. <i>Fluid Phase Equilibria</i> , 2020 , 518, 112625	2.5	5
51	Molecular dynamics simulation of CO-switchable surfactant regulated reversible emulsification/demulsification processes of a dodecane-saline system. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 23574-23585	3.6	5
50	Stoichiometry-Controlled Chirality Induced by Co-assembly of Tetraphenylethylene Derivative, ECD, and Water-Soluble Pillar[5]arene.. <i>ACS Applied Bio Materials</i> , 2021 , 4, 2066-2072	4.1	5
49	Transport Properties of Fe ₂ SiO ₄ Melt at High Pressure From Classical Molecular Dynamics: Implications for the Lifetime of the Magma Ocean. <i>Journal of Geophysical Research: Solid Earth</i> , 2018 , 123, 3667-3679	3.6	5
48	Complexation of quinone species on 2:1 dioctahedral phyllosilicate surfaces. <i>Applied Clay Science</i> , 2018 , 162, 268-275	5.2	5
47	Interstratification of graphene-like carbon layers within black talc from Southeastern China: Implications to sedimentary talc formation. <i>American Mineralogist</i> , 2016 , 101, 1668-1678	2.9	4
46	Uranyl Arsenate Complexes in Aqueous Solution: Insights from First-Principles Molecular Dynamics Simulations. <i>Inorganic Chemistry</i> , 2018 , 57, 5801-5809	5.1	4
45	Compensation phenomena found in <i>Acidithiobacillus ferrooxidans</i> after starvation stress. <i>Journal of Basic Microbiology</i> , 2014 , 54, 598-606	2.7	4
44	Nano-texture of penetrative foliation in metamorphic rocks. <i>Science in China Series D: Earth Sciences</i> , 2008 , 51, 1750-1758		4
43	Variation in surface energy heterogeneity of graphite due to adsorption of polyoxyethylene sorbitan monooleate. <i>Journal of Colloid and Interface Science</i> , 2004 , 280, 98-101	9.3	4
42	Discovery and analysis of ultra-micro grinding grain texture in slipping lamellae of ductile-brittle zone. <i>Science in China Series D: Earth Sciences</i> , 2004 , 47, 265		4
41	Coordination of Zr ⁴⁺ /Hf ⁴⁺ /Nb ⁵⁺ /Ta ⁵⁺ in silicate melts: insight from first principles molecular dynamics simulations. <i>Chemical Geology</i> , 2020 , 555, 119814	4.2	4
40	Thermodynamics of mixing in an isostructural solid solution: Simulation methodologies and application to the rutile-cassiterite system. <i>American Mineralogist</i> , 2016 , 101, 1197-1206	2.9	4
39	Mixed Coordination Silica at Megabar Pressure. <i>Physical Review Letters</i> , 2021 , 126, 035701	7.4	4
38	Petrogenesis of the Late Jurassic Laomengshan rhyodacite (Southeast China): constraints from zircon U-Pb dating, geochemistry and Sr-Nd-Ba-Hf isotopes. <i>International Geology Review</i> , 2014 , 56, 1964-1983	2.3	3
37	Monte Carlo study of argon adsorption energy on goethite (0 1 0) facet. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2006 , 281, 51-57	5.1	3
36	Study of influence on the surface energy heterogeneity of multiwalled carbon nanotubes after the adsorption of poly(acrylic acid). <i>Journal of Colloid and Interface Science</i> , 2004 , 278, 299-303	9.3	3
35	Enhanced Fluoride Uptake by Layered Double Hydroxides under Alkaline Conditions: Solid-State NMR Evidence of the Role of Surface >MgOH Sites. <i>Environmental Science & Technology</i> , 2021 , 55, 15082-15089	10.3	3

34	Examining geodetic glacier mass balance in the eastern Pamir transition zone. <i>Journal of Glaciology</i> , 2020 , 66, 927-937	3.4	3
33	Analysis of the <i>Talaromyces flavus</i> exometabolome reveals the complex responses of the fungus to minerals. <i>Geochimica Et Cosmochimica Acta</i> , 2021 , 298, 70-86	5.5	3
32	Sn(II) chloride speciation and equilibrium Sn isotope fractionation under hydrothermal conditions: A first principles study. <i>Geochimica Et Cosmochimica Acta</i> , 2021 , 300, 25-43	5.5	3
31	Redox potentials of aryl derivatives from hybrid functional based first principles molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 14911-7	3.6	3
30	Interfacial structures and acidity constants of goethite from first principles molecular dynamics simulations. <i>American Mineralogist</i> , 2021 ,	2.9	3
29	Thermodynamic properties of calcium ferrite-type MgAl ₂ O ₄ : A first principles study. <i>Science China Earth Sciences</i> , 2016 , 59, 831-839	4.6	2
28	A molecular dynamics study of uranyl-carbonate complexes adsorbed on basal surfaces of clay minerals. <i>Diqiu Huaxue</i> , 2015 , 34, 143-155		2
27	Comment on Empirical partition coefficients for Sr and Ca in marine barite: Implications for reconstructing seawater Sr and Ca concentrations by Kristen B. Averyt and Adina Paytan. <i>Geochemistry, Geophysics, Geosystems</i> , 2007 , 8, n/a-n/a	3.6	2
26	Monte Carlo simulations of surface energy of the open tetrahedral surface of 2:1-type phyllosilicate. <i>Journal of Colloid and Interface Science</i> , 2007 , 307, 17-23	9.3	2
25	Adsorption Behaviour of Tween80 on Graphite. <i>Adsorption Science and Technology</i> , 2005 , 23, 27-35	3.6	2
24	Changes in surface heterogeneity of multi-walled carbon nanotubes due to adsorption of poly(acrylic acid) by derivative isotherm summation method. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2005 , 264, 219-223	5.1	2
23	Variation in surface fractal of graphite due to the adsorption of polyoxyethylene sorbitan monooleate. <i>Applied Surface Science</i> , 2005 , 240, 244-250	6.7	2
22	Closest-Packing Water Monolayer Stably Intercalated in Phyllosilicate Minerals under High Pressure. <i>Langmuir</i> , 2020 , 36, 618-627	4	2
21	Emulation of short-range ordering within the Compound Energy Formalism: Application to the calcite-magnesite solid solution. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019 , 64, 115-125	1.9	2
20	A molecular dynamics study of Li speciation in hydrothermal fluids and silicate melts. <i>Chemical Geology</i> , 2021 , 584, 120528	4.2	2
19	First-principles study of high-pressure elasticity of CF- and CT-structure MgAl ₂ O ₄ . <i>Geophysical Research Letters</i> , 2012 , 39, n/a-n/a	4.9	1
18	Highly Zn, Mn-rich calcite in calcareous tufa from the Qixiashan Pb-Zn Mine, Nanjing: a possible candidate for Zn-Mn removal from mining impacted waters. <i>Science Bulletin</i> , 2009 , 54, 1376-1383	10.6	1
17	Cataclastic rheology of carbonate rocks. <i>Science in China Series D: Earth Sciences</i> , 2005 , 48, 1227-1233		1

16	Surface Acidity and As(V) Complexation of Iron Oxyhydroxides: Insights from First-Principles Molecular Dynamics Simulations. <i>Environmental Science & Technology</i> , 2021 , 55, 15921-15928	10.3	1
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