

# Xiancai Lu

## List of Publications by Year in Descending Order

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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	Superionic Silica-Water and Silica-Hydrogen Compounds in the Deep Interiors of Uranus and Neptune.. <i>Physical Review Letters</i> , <b>2022</b> , 128, 035702	7.4	6
158	Modified LB model for simulation of gas flow in shale pore systems by introducing end effects and local effective mean free path. <i>Journal of Petroleum Science and Engineering</i> , <b>2022</b> , 212, 110285	4.4	1
157	A MOLECULAR DYNAMICS SIMULATION STUDY OF Fe-CONTAINING PLYGORSKITE. <i>Clays and Clay Minerals</i> , <b>2021</b> , 69, 399-405	2.1	0
156	Surface Acidity and As(V) Complexation of Iron Oxyhydroxides: Insights from First-Principles Molecular Dynamics Simulations. <i>Environmental Science &amp; Technology</i> , <b>2021</b> , 55, 15921-15928	10.3	1
155	Mineral foraging and etching by the fungus <i>Talaromyces flavus</i> to obtain structurally bound iron. <i>Chemical Geology</i> , <b>2021</b> , 586, 120592	4.2	0
154	Enhanced Fluoride Uptake by Layered Double Hydroxides under Alkaline Conditions: Solid-State NMR Evidence of the Role of Surface >MgOH Sites. <i>Environmental Science &amp; Technology</i> , <b>2021</b> , 55, 15082-15089	10.3	3
153	Analysis of the <i>Talaromyces flavus</i> exometabolome reveals the complex responses of the fungus to minerals. <i>Geochimica Et Cosmochimica Acta</i> , <b>2021</b> , 298, 70-86	5.5	3
152	Sn(II) chloride speciation and equilibrium Sn isotope fractionation under hydrothermal conditions: A first principles study. <i>Geochimica Et Cosmochimica Acta</i> , <b>2021</b> , 300, 25-43	5.5	3
151	Stoichiometry-Controlled Chirality Induced by Co-assembly of Tetraphenylethylene Derivative, ECD, and Water-Soluble Pillar[5]arene.. <i>ACS Applied Bio Materials</i> , <b>2021</b> , 4, 2066-2072	4.1	5
150	Facet-Dependent Photodegradation of Methylene Blue by Hematite Nanoplates in Visible Light. <i>Environmental Science &amp; Technology</i> , <b>2021</b> , 55, 677-688	10.3	26
149	Selection of Planar Chiral Conformations between Pillar[5,6]arenes Induced by Amino Acid Derivatives in Aqueous Media. <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 5890-5896	4.8	10
148	Mixed Coordination Silica at Megabar Pressure. <i>Physical Review Letters</i> , <b>2021</b> , 126, 035701	7.4	4
147	Interfacial structures and acidity constants of goethite from first principles molecular dynamics simulations. <i>American Mineralogist</i> , <b>2021</b> ,	2.9	3
146	A molecular dynamics study of Li speciation in hydrothermal fluids and silicate melts. <i>Chemical Geology</i> , <b>2021</b> , 584, 120528	4.2	2
145	Writable and Self-Erasable Hydrogel Based on Dissipative Assembly Process from Multiple Carboxyl Tetraphenylethylene Derivative <b>2020</b> , 2, 425-429		18
144	Lattice Boltzmann Simulations on Shale Gas Flow in Slit Micro/Nanopores in Kerogen and Prediction of Cut Off Pore Throat. <i>Energy &amp; Fuels</i> , <b>2020</b> , 34, 15995-16005	4.1	1
143	A molecular dynamics simulation study of KF and NaF ion pairs in hydrothermal fluids. <i>Fluid Phase Equilibria</i> , <b>2020</b> , 518, 112625	2.5	5

142	A combined first principles and classical molecular dynamics study of clay-soil organic matters (SOMs) interactions. <i>Geochimica Et Cosmochimica Acta</i> , <b>2020</b> , 291, 110-125	5.5	14
141	Mountain biodiversity and ecosystem functions: interplay between geology and contemporary environments. <i>ISME Journal</i> , <b>2020</b> , 14, 931-944	11.9	33
140	Closest-Packing Water Monolayer Stably Intercalated in Phyllosilicate Minerals under High Pressure. <i>Langmuir</i> , <b>2020</b> , 36, 618-627	4	2
139	Molecular dynamics simulation of CO-switchable surfactant regulated reversible emulsification/demulsification processes of a dodecane-saline system. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 23574-23585	3.6	5
138	Nucleation and Growth of Crystal on a Substrate Surface: Structure Matching at the Atomistic Level. <i>ACS Symposium Series</i> , <b>2020</b> , 295-310	0.4	1
137	Coupling between clay swelling/collapse and cationic partition. <i>Geochimica Et Cosmochimica Acta</i> , <b>2020</b> , 285, 78-99	5.5	14
136	Diffusion of noble gases in subduction zone hydrous minerals. <i>Geochimica Et Cosmochimica Acta</i> , <b>2020</b> , 291, 50-61	5.5	0
135	Examining geodetic glacier mass balance in the eastern Pamir transition zone. <i>Journal of Glaciology</i> , <b>2020</b> , 66, 927-937	3.4	3
134	Coordination of Zr <sup>4+</sup> /Hf <sup>4+</sup> /Nb <sup>5+</sup> /Ta <sup>5+</sup> in silicate melts: insight from first principles molecular dynamics simulations. <i>Chemical Geology</i> , <b>2020</b> , 555, 119814	4.2	4
133	Anionic effect on nanostructure and morphology of bio-schwertmannite dynamically produced within cellular reproduction. <i>Nanomaterials and Nanotechnology</i> , <b>2020</b> , 10, 184798042095755	2.9	0
132	On the thermodynamics and kinetics of scorodite dissolution. <i>Geochimica Et Cosmochimica Acta</i> , <b>2019</b> , 265, 468-477	5.5	5
131	Mediation of Extracellular Polymeric Substances in Microbial Reduction of Hematite by MR-1. <i>Frontiers in Microbiology</i> , <b>2019</b> , 10, 575	5.7	20
130	First-Principles Study of Thermodynamics and Spin Transition in FeSiO <sub>3</sub> Liquid at High Pressure. <i>Geophysical Research Letters</i> , <b>2019</b> , 46, 3706-3716	4.9	5
129	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> , <b>2019</b> , 670, 1008-1018	10.2	5
128	Distribution and Mobility of Crude Oil-Brine in Clay Mesopores: Insights from Molecular Dynamics Simulations. <i>Langmuir</i> , <b>2019</b> , 35, 14818-14832	4	7
127	Understanding the Heterogeneous Nucleation of Heavy Metal Phyllosilicates on Clay Edges with First-Principles Molecular Dynamics. <i>Environmental Science &amp; Technology</i> , <b>2019</b> , 53, 13704-13712	10.3	8
126	Synthesis of 2D Hexagonal Hematite Nanosheets and the Crystal Growth Mechanism. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 16727-16735	5.1	14
125	An atomic-scale understanding of the initial stage of nucleation of heavy metal cations on clay edges. <i>Geochimica Et Cosmochimica Acta</i> , <b>2019</b> , 248, 161-171	5.5	8

124	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> , <b>2019</b> , 64, 115-125	1.9	2
123	Specificity of low molecular weight organic acids on the release of elements from lizardite during fungal weathering. <i>Geochimica Et Cosmochimica Acta</i> , <b>2019</b> , 256, 20-34	5.5	9
122	Complexation of heavy metal cations on clay edges at elevated temperatures. <i>Chemical Geology</i> , <b>2018</b> , 479, 36-46	4.2	13
121	Structural Incorporation of Manganese into Goethite and Its Enhancement of Pb(II) Adsorption. <i>Environmental Science &amp; Technology</i> , <b>2018</b> , 52, 4719-4727	10.3	40
120	Regulates Biofilm Development of MnB1 as a Primary Response to HO and Mn. <i>Frontiers in Microbiology</i> , <b>2018</b> , 9, 1490	5.7	11
119	Uranyl Arsenate Complexes in Aqueous Solution: Insights from First-Principles Molecular Dynamics Simulations. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 5801-5809	5.1	4
118	Influences of Cation Ratio, Anion Type, and Water Content on Polytypism of Layered Double Hydroxides. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 7299-7313	5.1	13
117	Thermoelastic Properties of Aluminous Phases in MORB From First-Principle Calculation: Implications for Earth's Lower Mantle. <i>Journal of Geophysical Research: Solid Earth</i> , <b>2018</b> , 123, 10,583	3.6	1
116	Collaborative effects of Acidithiobacillus ferrooxidans and ferrous ions on the oxidation of chalcopyrite. <i>Chemical Geology</i> , <b>2018</b> , 493, 109-120	4.2	24
115	Transport Properties of Fe <sub>2</sub> SiO <sub>4</sub> Melt at High Pressure From Classical Molecular Dynamics: Implications for the Lifetime of the Magma Ocean. <i>Journal of Geophysical Research: Solid Earth</i> , <b>2018</b> , 123, 3667-3679	3.6	5
114	Complexation of quinone species on 2:1 dioctahedral phyllosilicate surfaces. <i>Applied Clay Science</i> , <b>2018</b> , 162, 268-275	5.2	5
113	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> , <b>2017</b> , 203, 54-68	5.5	41
112	Molecular simulation study on K <sup>+</sup> Cl <sup>-</sup> ion pair in geological fluids. <i>Acta Geochimica</i> , <b>2017</b> , 36, 1-8	2.2	15
111	Thermodynamic properties in the Fe(II)-Fe(III)-As(V)-HClO <sub>4</sub> -H <sub>2</sub> O and Fe(II)-Fe(III)-As(V)-HCl-H <sub>2</sub> O systems from 5 to 90 °C. <i>Chemical Geology</i> , <b>2017</b> , 460, 37-45	4.2	6
110	Geochemical fates and unusual distribution of arsenic in natural ferromanganese duricrust. <i>Applied Geochemistry</i> , <b>2017</b> , 76, 74-87	3.5	7
109	Complexation of carboxylate on smectite surfaces. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 18400-18406	3.8	11
108	Nanogeosciences: Research History, Current Status, and Development Trends. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2017</b> , 17, 5930-5965	1.3	60
107	Structure, acidity, and metal complexing properties of oxythioarsenites in hydrothermal solutions. <i>Chemical Geology</i> , <b>2017</b> , 471, 131-140	4.2	0

106	Molecular Dynamics Simulation of Alkylammonium-Intercalated Vermiculites. <i>Clays and Clay Minerals</i> , <b>2017</b> , 65, 378-386	2.1	7
105	Oxidation and Mineralization of Mn <sup>2+</sup> Ions Mediated by <i>Pseudomonas putida</i> : Insights from an Experimental Study. <i>Acta Geologica Sinica</i> , <b>2017</b> , 91, 1276-1285	0.7	7
104	Interlayer Structures and Dynamics of Arsenate and Arsenite Intercalated Layered Double Hydroxides: A First Principles Study. <i>Minerals (Basel, Switzerland)</i> , <b>2017</b> , 7, 53	2.4	5
103	Studies on Micro/Nano-Sized Grinding Grains on Shear-Slip Surfaces in Rocks. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2017</b> , 17, 7069-7075	1.3	1
102	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> , <b>2016</b> , 33, 118-134	2.5	17
101	Interstratification of graphene-like carbon layers within black talc from Southeastern China: Implications to sedimentary talc formation. <i>American Mineralogist</i> , <b>2016</b> , 101, 1668-1678	2.9	4
100	Cadmium(II) Complexes Adsorbed on Clay Edge Surfaces: Insight from First Principles Molecular Dynamics Simulation. <i>Clays and Clay Minerals</i> , <b>2016</b> , 64, 337-347	2.1	27
99	A rapid glacier surge on Mount Tobe Feng, western China, 2015. <i>Journal of Glaciology</i> , <b>2016</b> , 62, 407-409	3.4	12
98	Jumping Diffusion of Water Intercalated in Layered Double Hydroxides. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 12924-12931	3.8	14
97	Thermodynamic properties of calcium ferrite-type MgAl <sub>2</sub> O <sub>4</sub> : A first principles study. <i>Science China Earth Sciences</i> , <b>2016</b> , 59, 831-839	4.6	2
96	Confined water in tunnel nanopores of sepiolite: Insights from molecular simulations. <i>American Mineralogist</i> , <b>2016</b> , 101, 713-718	2.9	10
95	Surface Wettability of Basal Surfaces of Clay Minerals: Insights from Molecular Dynamics Simulation. <i>Energy &amp; Fuels</i> , <b>2016</b> , 30, 149-160	4.1	70
94	Changes in the Interlayer Structure and Thermodynamics of Hydrated Montmorillonite Under Basin Conditions: Molecular Simulation Approaches. <i>Clays and Clay Minerals</i> , <b>2016</b> , 64, 503-511	2.1	6
93	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> , <b>2016</b> , 160-161, 1-10	5.5	36
92	Redox potentials of aryl derivatives from hybrid functional based first principles molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 14911-7	3.6	3
91	Thermodynamics of mixing in an isostructural solid solution: Simulation methodologies and application to the rutile-cassiterite system. <i>American Mineralogist</i> , <b>2016</b> , 101, 1197-1206	2.9	4
90	Acidity constants and redox potentials of uranyl ions in hydrothermal solutions. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 26040-26048	3.6	10
89	Structures and Acidity Constants of Silver-Sulfide Complexes in Hydrothermal Fluids: A First-Principles Molecular Dynamics Study. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 8435-8443	2.8	6

88	Slow dynamics of water confined in Newton black films. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 19183-93	3.6	10
87	Temperature dependence of interfacial structures and acidity of clay edge surfaces. <i>Geochimica Et Cosmochimica Acta</i> , <b>2015</b> , 160, 91-99	5.5	20
86	Structures and acidity constants of arsenite and thioarsenite species in hydrothermal solutions. <i>Chemical Geology</i> , <b>2015</b> , 411, 192-199	4.2	13
85	Interfacial structures and acidity of edge surfaces of ferruginous smectites. <i>Geochimica Et Cosmochimica Acta</i> , <b>2015</b> , 168, 293-301	5.5	25
84	A molecular dynamics study of uranyl-carbonate complexes adsorbed on basal surfaces of clay minerals. <i>Diqiu Huaxue</i> , <b>2015</b> , 34, 143-155		2
83	Molecular simulation study of hydrated Na-rectorite. <i>Langmuir</i> , <b>2015</b> , 31, 2008-13	4	12
82	Helium diffusion in olivine based on first principles calculations. <i>Geochimica Et Cosmochimica Acta</i> , <b>2015</b> , 156, 145-153	5.5	15
81	Secondary minerals of weathered orpiment-realgar-bearing tailings in Shimen carbonate-type realgar mine, Changde, Central China. <i>Mineralogy and Petrology</i> , <b>2015</b> , 109, 1-15	1.6	31
80	Atomistic simulation on mixing thermodynamics of calcite-smithsonite solid solutions. <i>American Mineralogist</i> , <b>2015</b> , 100, 172-180	2.9	5
79	Petrogenesis of the Late Jurassic Laomengshan rhyodacite (Southeast China): constraints from zircon U/Bb dating, geochemistry and Sr/Nd/Pb/Bi isotopes. <i>International Geology Review</i> , <b>2014</b> , 56, 1964-1983	2.3	3
78	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> , <b>2014</b> , 30, 10600-4		19
77	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> , <b>2014</b> , 118, 19205-19213	3.8	13
76	Reduction of jarosite by <i>Shewanella oneidensis</i> MR-1 and secondary mineralization. <i>Geochimica Et Cosmochimica Acta</i> , <b>2014</b> , 124, 54-71	5.5	37
75	Quantitative X-ray photoelectron spectroscopy-based depth profiling of bioleached arsenopyrite surface by <i>Acidithiobacillus ferrooxidans</i> . <i>Geochimica Et Cosmochimica Acta</i> , <b>2014</b> , 127, 120-139	5.5	49
74	Surface acidity of 2:1-type dioctahedral clay minerals from first principles molecular dynamics simulations. <i>Geochimica Et Cosmochimica Acta</i> , <b>2014</b> , 140, 410-417	5.5	63
73	Hydration and Mobility of Interlayer Ions of (Nax, Cay)-Montmorillonite: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 29811-29821	3.8	63
72	Surface acidity of quartz: understanding the crystallographic control. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 26909-16	3.6	35
71	Compensation phenomena found in <i>Acidithiobacillus ferrooxidans</i> after starvation stress. <i>Journal of Basic Microbiology</i> , <b>2014</b> , 54, 598-606	2.7	4

70	Understanding surface acidity of gibbsite with first principles molecular dynamics simulations. <i>Geochimica Et Cosmochimica Acta</i> , <b>2013</b> , 120, 487-495	5.5	46
69	Analysis of Genes and Proteins in <i>Acidithiobacillus ferrooxidans</i> During Growth and Attachment on Pyrite Under Different Conditions. <i>Geomicrobiology Journal</i> , <b>2013</b> , 30, 255-267	2.5	8
68	Acidity of edge surface sites of montmorillonite and kaolinite. <i>Geochimica Et Cosmochimica Acta</i> , <b>2013</b> , 117, 180-190	5.5	146
67	Bioleaching of chalcopyrite by <i>Acidithiobacillus ferrooxidans</i> . <i>Minerals Engineering</i> , <b>2013</b> , 53, 184-192	4.9	19
66	Mineralogical characteristics of unusual black talc ores in Guangfeng County, Jiangxi Province, China. <i>Applied Clay Science</i> , <b>2013</b> , 74, 37-46	5.2	15
65	Solution Structures and Acidity Constants of Molybdic Acid. <i>Journal of Physical Chemistry Letters</i> , <b>2013</b> , 4, 2926-2930	6.4	33
64	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/Pb/Hf isotopes. <i>International Geology Review</i> , <b>2013</b> , 55, 1220-1238	2.3	19
63	Molecular Dynamics Simulation of the Effects of NaCl on Electrostatic Properties of Newton Black Films. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 21913-21922	3.8	15
62	Microbial Oxidation of Sulfide Tailings and the Environmental Consequences. <i>Elements</i> , <b>2012</b> , 8, 119-124	3.8	54
61	First-principles molecular dynamics study of stepwise hydrolysis reactions of Y <sup>3+</sup> + cations. <i>Chemical Geology</i> , <b>2012</b> , 334, 37-43	4.2	9
60	Constraints on timing and origin of the Dayinjian intrusion and associated molybdenum mineralization, western Dabie orogen, central China. <i>International Geology Review</i> , <b>2012</b> , 54, 1579-1596	2.3	15
59	Interlayer Structure and Dynamics of HDTMA <sup>+</sup> -Intercalated Rectorite with and without Water: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 13071-13078	3.8	18
58	Silver speciation in chloride-containing hydrothermal solutions from first principles molecular dynamics simulations. <i>Chemical Geology</i> , <b>2012</b> , 294-295, 103-112	4.2	30
57	Atomic-scale structures of interfaces between phyllosilicate edges and water. <i>Geochimica Et Cosmochimica Acta</i> , <b>2012</b> , 81, 56-68	5.5	54
56	Atomic scale structures of interfaces between kaolinite edges and water. <i>Geochimica Et Cosmochimica Acta</i> , <b>2012</b> , 92, 233-242	5.5	38
55	First-principles study of high-pressure elasticity of CF- and CT-structure MgAl <sub>2</sub> O <sub>4</sub> . <i>Geophysical Research Letters</i> , <b>2012</b> , 39, n/a-n/a	4.9	1
54	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> , <b>2012</b> , 24, 234-247	3.2	16
53	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 Mine in Eastern China. <i>Geomicrobiology Journal</i> , <b>2012</b> , 29, 274-286	2.5	14

52	First-Principles Molecular Dynamics Insight into Fe <sup>2+</sup> Complexes Adsorbed on Edge Surfaces of Clay Minerals. <i>Clays and Clay Minerals</i> , <b>2012</b> , 60, 341-347	2.1	9
51	Effects of CO <sub>2</sub> adsorption on coal deformation during geological sequestration. <i>Journal of Geophysical Research</i> , <b>2011</b> , 116,		34
50	Speciation of gold in hydrosulphide-rich ore-forming fluids: Insights from first-principles molecular dynamics simulations. <i>Geochimica Et Cosmochimica Acta</i> , <b>2011</b> , 75, 185-194	5.5	35
49	Acidities of confined water in interlayer space of clay minerals. <i>Geochimica Et Cosmochimica Acta</i> , <b>2011</b> , 75, 4978-4986	5.5	22
48	Porphyry and skarn Au-Cu deposits in the Shizishan orefield, Tongling, East China: U-Pb dating and in-situ Hf isotope analysis of zircons and petrogenesis of associated granitoids. <i>Ore Geology Reviews</i> , <b>2011</b> , 43, 182-193	3.2	26
47	Solvation forces between molecularly rough surfaces. <i>Journal of Colloid and Interface Science</i> , <b>2011</b> , 362, 382-8	9.3	21
46	Anorthite dissolution promoted by bacterial adhesion: Direct evidence from dialytic experiment. <i>Science China Earth Sciences</i> , <b>2011</b> , 54, 204-211	4.6	5
45	Understanding hydration of Zn <sup>2+</sup> in hydrothermal fluids with ab initio molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 13305-9	3.6	20
44	Hydration of methane intercalated in Na-smectites with distinct layer charge: insights from molecular simulations. <i>Journal of Colloid and Interface Science</i> , <b>2011</b> , 355, 237-42	9.3	47
43	Deformation of Coal Induced by Methane Adsorption at Geological Conditions. <i>Energy &amp; Fuels</i> , <b>2010</b> , 24, 5955-5964	4.1	69
42	In silico calculation of acidity constants of carbonic acid conformers. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 12914-7	2.8	14
41	Acid dissociation mechanisms of Si(OH) <sub>4</sub> and Al(H <sub>2</sub> O) <sub>6</sub> <sup>3+</sup> in aqueous solution. <i>Geochimica Et Cosmochimica Acta</i> , <b>2010</b> , 74, 510-516	5.5	35
40	Material Properties of Marine Hydrogenous Ferromanganese Crust and Its Performance in Desulfurization. <i>Acta Geologica Sinica</i> , <b>2010</b> , 80, 441-450	0.7	
39	Ab Initio Molecular Dynamics Study of Fe-Containing Smectites. <i>Clays and Clay Minerals</i> , <b>2010</b> , 58, 89-96	2.1	12
38	Hydration mechanisms of Cu(2+): tetra-, penta- or hexa-coordinated?. <i>Physical Chemistry Chemical Physics</i> , <b>2010</b> , 12, 10801-4	3.6	39
37	Roles of adhered <i>Paenibacillus polymyxa</i> in the dissolution and flotation of bauxite: a dialytic investigation. <i>Frontiers of Earth Science</i> , <b>2010</b> , 4, 167-173		5
36	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> , <b>2010</b> , 36, 1339-1344	4.5	18
35	Molecular dynamics insight into the cointercalation of hexadecyltrimethyl-ammonium and acetate ions into smectites. <i>American Mineralogist</i> , <b>2009</b> , 94, 143-150	2.9	46



34	Development of online instructional resources for Earth system science education: An example of current practice from China. <i>Computers and Geosciences</i> , <b>2009</b> , 35, 1271-1279	4.5	8
33	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> , <b>2009</b> , 54, 1376-1383	10.6	1
32	Source rocks in Mesozoic-Cenozoic continental rift basins, east China: A case from Dongying Depression, Bohai Bay Basin. <i>Organic Geochemistry</i> , <b>2009</b> , 40, 229-242	3.1	70
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