

Xiancai Lu

List of Publications by Year in descending order

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161
papers

3,740
citations

126858

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162
docs citations

162
times ranked

3418
citing authors

#	ARTICLE	IF	CITATIONS
1	Acidity of edge surface sites of montmorillonite and kaolinite. <i>Geochimica Et Cosmochimica Acta</i> , 2013, 117, 180-190.	1.6	180
2	A Thermodynamic Understanding of Clay-Swelling Inhibition by Potassium Ions. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 6300-6303.	7.2	118
3	Surface Wettability of Basal Surfaces of Clay Minerals: Insights from Molecular Dynamics Simulation. <i>Energy & Fuels</i> , 2016, 30, 149-160.	2.5	101
4	Source rocks in Mesozoicâ€Cenozoic continental rift basins, east China: A case from Dongying Depression, Bohai Bay Basin. <i>Organic Geochemistry</i> , 2009, 40, 229-242.	0.9	93
5	Hydration and Mobility of Interlayer Ions of (Na _x) ₁ ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 587 Td (Ca _x) ₁ C, 2014, 118, 29811-29821.	1.5	93
6	Deformation of Coal Induced by Methane Adsorption at Geological Conditions. <i>Energy & Fuels</i> , 2010, 24, 5955-5964.	2.5	82
7	Effects of layer-charge distribution on the thermodynamic and microscopic properties of Cs-smectite. <i>Geochimica Et Cosmochimica Acta</i> , 2008, 72, 1837-1847.	1.6	75
8	Structural Incorporation of Manganese into Goethite and Its Enhancement of Pb(II) Adsorption. <i>Environmental Science & Technology</i> , 2018, 52, 4719-4727.	4.6	74
9	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.	1.6	72
10	Nanogeosciences: Research History, Current Status, and Development Trends. <i>Journal of Nanoscience and Nanotechnology</i> , 2017, 17, 5930-5965.	0.9	67
11	Facet-Dependent Photodegradation of Methylene Blue by Hematite Nanoplates in Visible Light. <i>Environmental Science & Technology</i> , 2021, 55, 677-688.	4.6	67
12	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.	0.6	66
13	Microbial Oxidation of Sulfide Tailings and the Environmental Consequences. <i>Elements</i> , 2012, 8, 119-124.	0.5	65
14	Mountain biodiversity and ecosystem functions: interplay between geology and contemporary environments. <i>ISME Journal</i> , 2020, 14, 931-944.	4.4	64
15	Atomic-scale structures of interfaces between phyllosilicate edges and water. <i>Geochimica Et Cosmochimica Acta</i> , 2012, 81, 56-68.	1.6	63
16	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.	1.6	63
17	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.	1.6	63
18	Reduction of jarosite by <i>Shewanella oneidensis</i> MR-1 and secondary mineralization. <i>Geochimica Et Cosmochimica Acta</i> , 2014, 124, 54-71.	1.6	62

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19	Understanding surface acidity of gibbsite with first principles molecular dynamics simulations. <i>Geochimica Et Cosmochimica Acta</i> , 2013, 120, 487-495.	1.6	61
20	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.	1.9	57
21	Surface acidity of quartz: understanding the crystallographic control. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26909-26916.	1.3	52
22	Atomic scale structures of interfaces between kaolinite edges and water. <i>Geochimica Et Cosmochimica Acta</i> , 2012, 92, 233-242.	1.6	51
23	Molecular dynamics insight into the cointercalation of hexadecyltrimethyl-ammonium and acetate ions into smectites. <i>American Mineralogist</i> , 2009, 94, 143-150.	0.9	49
24	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, 237-242.	5.0	49
25	Hydration mechanisms of Cu ²⁺ : tetra-, penta- or hexa-coordinated?. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10801.	1.3	45
26	Effects of CO ₂ adsorption on coal deformation during geological sequestration. <i>Journal of Geophysical Research</i> , 2011, 116, .	3.3	41
27	Solution Structures and Acidity Constants of Molybdic Acid. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2926-2930.	2.1	39
28	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.	1.6	38
29	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.	1.6	38
30	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.	0.4	38
31	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> , 2011, 43, 182-193.	1.1	36
32	Sorption and Desorption of Phenanthrene onto Iron, Copper, and Silicon Dioxide Nanoparticles. <i>Langmuir</i> , 2008, 24, 10929-10935.	1.6	35
33	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.	1.6	34
34	Interfacial structures and acidity of edge surfaces of ferruginous smectites. <i>Geochimica Et Cosmochimica Acta</i> , 2015, 168, 293-301.	1.6	34
35	Writable and Self-Erasable Hydrogel Based on Dissipative Assembly Process from Multiple Carboxyl Tetraphenylethylene Derivative. , 2020, 2, 425-429.		34
36	Silver speciation in chloride-containing hydrothermal solutions from first principles molecular dynamics simulations. <i>Chemical Geology</i> , 2012, 294-295, 103-112.	1.4	33

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37	Acidities of confined water in interlayer space of clay minerals. <i>Geochimica Et Cosmochimica Acta</i> , 2011, 75, 4978-4986.	1.6	32
38	Synthesis of 2D Hexagonal Hematite Nanosheets and the Crystal Growth Mechanism. <i>Inorganic Chemistry</i> , 2019, 58, 16727-16735.	1.9	32
39	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.	0.6	31
40	Collaborative effects of <i>Acidithiobacillus ferrooxidans</i> and ferrous ions on the oxidation of chalcopyrite. <i>Chemical Geology</i> , 2018, 493, 109-120.	1.4	31
41	bifA Regulates Biofilm Development of <i>Pseudomonas putida</i> MnB1 as a Primary Response to H ₂ O ₂ and Mn ²⁺ . <i>Frontiers in Microbiology</i> , 2018, 9, 1490.	1.5	31
42	Mediation of Extracellular Polymeric Substances in Microbial Reduction of Hematite by <i>Shewanella oneidensis</i> MR-1. <i>Frontiers in Microbiology</i> , 2019, 10, 575.	1.5	31
43	Coupling between clay swelling/collapse and cationic partition. <i>Geochimica Et Cosmochimica Acta</i> , 2020, 285, 78-99.	1.6	29
44	Bioleaching of chalcopyrite by <i>Acidithiobacillus ferrooxidans</i> . <i>Minerals Engineering</i> , 2013, 53, 184-192.	1.8	28
45	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.	1.0	28
46	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.	1.6	28
47	Influences of Cation Ratio, Anion Type, and Water Content on Polyttypism of Layered Double Hydroxides. <i>Inorganic Chemistry</i> , 2018, 57, 7299-7313.	1.9	27
48	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.	1.7	26
49	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.	4.6	25
50	Understanding hydration of Zn ²⁺ in hydrothermal fluids with ab initio molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13305.	1.3	24
51	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, 10600-10607.	1.6	24
52	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.	2.0	23
53	Solvation forces between molecularly rough surfaces. <i>Journal of Colloid and Interface Science</i> , 2011, 362, 382-388.	5.0	23
54	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.	1.6	23

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55	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, .	1.5	22
56	Petrogenesis of the Bao'anhai 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> , 2013, 55, 1220-1238.	1.1	22
57	Temperature dependence of interfacial structures and acidity of clay edge surfaces. <i>Geochimica Et Cosmochimica Acta</i> , 2015, 160, 91-99.	1.6	22
58	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.	4.6	22
59	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.	1.5	21
60	Helium diffusion in olivine based on first principles calculations. <i>Geochimica Et Cosmochimica Acta</i> , 2015, 156, 145-153.	1.6	21
61	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.	1.9	20
62	Mixed Coordination Silica at Megabar Pressure. <i>Physical Review Letters</i> , 2021, 126, 035701.	2.9	20
63	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.	1.8	19
64	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.	0.4	19
65	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> , 2012, 29, 274-286.	1.0	19
66	Numerical modelling of the hydrocarbon generation of tertiary source rocks intruded by doleritic sills in the Zhanhua depression, Bohai Basin, China. <i>Basin Research</i> , 2012, 24, 234-247.	1.3	19
67	Mineralogical characteristics of unusual black talc ores in Guangfeng County, Jiangxi Province, China. <i>Applied Clay Science</i> , 2013, 74, 37-46.	2.6	19
68	Distribution and Mobility of Crude Oil-Brine in Clay Mesopores: Insights from Molecular Dynamics Simulations. <i>Langmuir</i> , 2019, 35, 14818-14832.	1.6	19
69	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.	1.6	19
70	Superionic Silica-Water and Silica-Hydrogen Compounds in the Deep Interiors of Uranus and Neptune. <i>Physical Review Letters</i> , 2022, 128, 035702.	2.9	19
71	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.	1.5	18
72	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.	1.5	18

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73	Jumping Diffusion of Water Intercalated in Layered Double Hydroxides. <i>Journal of Physical Chemistry C</i> , 2016, 120, 12924-12931.	1.5	18
74	Molecular simulation study on K+â€“Clâ” ion pair in geological fluids. <i>Acta Geochimica</i> , 2017, 36, 1-8.	0.7	18
75	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.	1.6	18
76	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.	1.1	16
77	Complexation of heavy metal cations on clay edges at elevated temperatures. <i>Chemical Geology</i> , 2018, 479, 36-46.	1.4	16
78	On the thermodynamics and kinetics of scorodite dissolution. <i>Geochimica Et Cosmochimica Acta</i> , 2019, 265, 468-477.	1.6	16
79	First-principles molecular dynamics study of stepwise hydrolysis reactions of Y3+ cations. <i>Chemical Geology</i> , 2012, 334, 37-43.	1.4	15
80	Molecular Simulation Study of Hydrated Na-Rectorite. <i>Langmuir</i> , 2015, 31, 2008-2013.	1.6	15
81	Confined water in tunnel nanopores of sepiolite: Insights from molecular simulations. <i>American Mineralogist</i> , 2016, 101, 713-718.	0.9	15
82	Complexation of carboxylate on smectite surfaces. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 18400-18406.	1.3	15
83	In Silico Calculation of Acidity Constants of Carbonic Acid Conformers. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12914-12917.	1.1	14
84	First-Principles Molecular Dynamics Insight into Fe²⁺ Complexes Adsorbed on Edge Surfaces of Clay Minerals. <i>Clays and Clay Minerals</i> , 2012, 60, 341-347.	0.6	14
85	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.	0.8	13
86	Structures and acidity constants of arsenite and thioarsenite species in hydrothermal solutions. <i>Chemical Geology</i> , 2015, 411, 192-199.	1.4	13
87	Acidity constants and redox potentials of uranyl ions in hydrothermal solutions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26040-26048.	1.3	13
88	A rapid glacier surge on Mount Tobe Feng, western China, 2015. <i>Journal of Glaciology</i> , 2016, 62, 407-409.	1.1	13
89	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.	3.9	13
90	Molecular dynamics simulation of CO₂-switchable surfactant regulated reversible emulsification/demulsification processes of a dodecaneâ€“saline system. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 23574-23585.	1.3	13

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91	A New Integrated Method for Characterizing Surface Energy Heterogeneity from a Single Adsorption Isotherm. <i>Journal of Physical Chemistry B</i> , 2005, 109, 15828-15834.	1.2	12
92	<i>Ab Initio</i> Molecular Dynamics Study of Fe-Containing Smectites. <i>Clays and Clay Minerals</i> , 2010, 58, 89-96.	0.6	12
93	Slow dynamics of water confined in Newton black films. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 19183-19193.	1.3	12
94	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.	0.9	11
95	The surface fractal investigation on carbon nanotubes modified by the adsorption of poly(acrylic) Tj ETQq1 1 0.784314 rgBT /Overlock 11	2.2	11
96	Stoichiometry-Controlled Chirality Induced by Co-assembly of Tetraphenylethylene Derivative, β -CD, and Water-Soluble Pillar[5]arene. <i>ACS Applied Bio Materials</i> , 2021, 4, 2066-2072.	2.3	11
97	A molecular dynamics simulation study of KF and NaF ion pairs in hydrothermal fluids. <i>Fluid Phase Equilibria</i> , 2020, 518, 112625.	1.4	11
98	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 Å°C. <i>Chemical Geology</i> , 2017, 460, 37-45.	1.4	10
99	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.	4.6	10
100	Discovery of low-mature hydrocarbon in manganese nodules and ooze from the Central Pacific deep sea floor. <i>Science Bulletin</i> , 2002, 47, 939.	1.7	9
101	A comparative study of natural and experimental nano-sized grinding grain textures in rocks. <i>Science Bulletin</i> , 2008, 53, 1217-1221.	4.3	9
102	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.	2.0	9
103	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.	1.0	9
104	Geochemical fates and unusual distribution of arsenic in natural ferromanganese duricrust. <i>Applied Geochemistry</i> , 2017, 76, 74-87.	1.4	9
105	Molecular Dynamics Simulation of Alkylammonium-Intercalated Vermiculites. <i>Clays and Clay Minerals</i> , 2017, 65, 378-386.	0.6	9
106	Uranyl Arsenate Complexes in Aqueous Solution: Insights from First-Principles Molecular Dynamics Simulations. <i>Inorganic Chemistry</i> , 2018, 57, 5801-5809.	1.9	9
107	Examining geodetic glacier mass balance in the eastern Pamir transition zone. <i>Journal of Glaciology</i> , 2020, 66, 927-937.	1.1	9
108	Atomistic simulation on mixing thermodynamics of calcite-smithsonite solid solutions. <i>American Mineralogist</i> , 2015, 100, 172-180.	0.9	8

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109	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.	0.6	8
110	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.	0.9	8
111	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.	0.8	8
112	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.	1.4	8
113	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.	1.6	8
114	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.	0.5	7
115	Anorthite dissolution promoted by bacterial adhesion: Direct evidence from dialytic experiment. <i>Science China Earth Sciences</i> , 2011, 54, 204-211.	2.3	7
116	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.	1.4	7
117	Closest-Packing Water Monolayer Stably Intercalated in Phyllosilicate Minerals under High Pressure. <i>Langmuir</i> , 2020, 36, 618-627.	1.6	7
118	Interfacial structures and acidity constants of goethite from first-principles Molecular Dynamics simulations. <i>American Mineralogist</i> , 2021, 106, 1736-1743.	0.9	7
119	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.	1.1	6
120	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.	0.9	6
121	Complexation of quinone species on 2:1 dioctahedral phyllosilicate surfaces. <i>Applied Clay Science</i> , 2018, 162, 268-275.	2.6	6
122	First-Principles Study of Thermodynamics and Spin Transition in FeSiO ₃ Liquid at High Pressure. <i>Geophysical Research Letters</i> , 2019, 46, 3706-3716.	1.5	6
123	Observation of ultra-microtexture of fault rocks in shearing-sliding zones*. <i>Progress in Natural Science: Materials International</i> , 2005, 15, 430-434.	1.8	5
124	Interlayer Structures and Dynamics of Arsenate and Arsenite Intercalated Layered Double Hydroxides: A First Principles Study. <i>Minerals (Basel, Switzerland)</i> , 2017, 7, 53.	0.8	5
125	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.	0.7	5
126	A molecular dynamics study of Li speciation in hydrothermal fluids and silicate melts. <i>Chemical Geology</i> , 2021, 584, 120528.	1.4	5

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127	Mineral foraging and etching by the fungus <i>Talaromyces flavus</i> to obtain structurally bound iron. <i>Chemical Geology</i> , 2021, 586, 120592.	1.4	5
128	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> , 2022, 212, 110285.	2.1	5
129	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.	5.0	4
130	Nano-texture of penetrative foliation in metamorphic rocks. <i>Science in China Series D: Earth Sciences</i> , 2008, 51, 1750-1758.	0.9	4
131	Compensation phenomena found in <i>Acidithiobacillus ferrooxidans</i> after starvation stress. <i>Journal of Basic Microbiology</i> , 2014, 54, 598-606.	1.8	4
132	Petrogenesis of the Late Jurassic Laomengshan rhyodacite (Southeast China): constraints from zircon U-Pb dating, geochemistry and Sr-Nd-Pb-Hf isotopes. <i>International Geology Review</i> , 2014, 56, 1964-1983.	1.1	4
133	Redox potentials of aryl derivatives from hybrid functional based first principles molecular dynamics. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 14911-14917.	1.3	4
134	Thermodynamic properties of calcium ferrite-type MgAl ₂ O ₄ : A first principles study. <i>Science China Earth Sciences</i> , 2016, 59, 831-839.	2.3	4
135	Thermoelastic Properties of Aluminous Phases in MORB from First Principles Calculation: Implications for Earth's Lower Mantle. <i>Journal of Geophysical Research: Solid Earth</i> , 2018, 123, 10,583.	1.4	4
136	Diffusion of noble gases in subduction zone hydrous minerals. <i>Geochimica Et Cosmochimica Acta</i> , 2020, 291, 50-61.	1.6	4
137	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.	0.9	4
138	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.	5.0	3
139	Monte Carlo study of argon adsorption energy on goethite (010) facet. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2006, 281, 51-57.	2.3	3
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