Xiandong Liu

List of Publications by Year in descending order

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64 papers	2,059 citations	236925 25 h-index	254184 43 g-index
68 all docs	68 docs citations	68 times ranked	1606 citing authors

#	Article	IF	Citations
1	Redox Potentials and Acidity Constants from Density Functional Theory Based Molecular Dynamics. Accounts of Chemical Research, 2014, 47, 3522-3529.	15.6	181
2	Acidity of edge surface sites of montmorillonite and kaolinite. Geochimica Et Cosmochimica Acta, 2013, 117, 180-190.	3.9	180
3	Surface Wettability of Basal Surfaces of Clay Minerals: Insights from Molecular Dynamics Simulation. Energy & Fuels, 2016, 30, 149-160.	5.1	101
4	Hydration and Mobility of Interlayer Ions of (Na_x,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 627 Td (Ca_y C, 2014, 118, 29811-29821.	3.1	93
5	Effects of layer-charge distribution on the thermodynamic and microscopic properties of Cs-smectite. Geochimica Et Cosmochimica Acta, 2008, 72, 1837-1847.	3.9	75
6	Surface acidity of 2:1-type dioctahedral clay minerals from first principles molecular dynamics simulations. Geochimica Et Cosmochimica Acta, 2014, 140, 410-417.	3.9	72
7	Interlayer Structure and Dynamics of Alkylammonium-intercalated Smectites with and without Water: A Molecular Dynamics Study. Clays and Clay Minerals, 2007, 55, 554-564.	1.3	66
8	Atomic-scale structures of interfaces between phyllosilicate edges and water. Geochimica Et Cosmochimica Acta, 2012, 81, 56-68.	3.9	63
9	Surface complexation of heavy metal cations on clay edges: insights from first principles molecular dynamics simulation of Ni(II). Geochimica Et Cosmochimica Acta, 2017, 203, 54-68.	3.9	63
10	Understanding surface acidity of gibbsite with first principles molecular dynamics simulations. Geochimica Et Cosmochimica Acta, 2013, 120, 487-495.	3.9	61
11	Surface acidity of quartz: understanding the crystallographic control. Physical Chemistry Chemical Physics, 2014, 16, 26909-26916.	2.8	52
12	Atomic scale structures of interfaces between kaolinite edges and water. Geochimica Et Cosmochimica Acta, 2012, 92, 233-242.	3.9	51
13	Molecular dynamics insight into the cointercalation of hexadecyltrimethyl-ammonium and acetate ions into smectites. American Mineralogist, 2009, 94, 143-150.	1.9	49
14	Mechanistic Understanding of Uranyl Ion Complexation on Montmorillonite Edges: A Combined First-Principles Molecular Dynamicsâ€“Surface Complexation Modeling Approach. Environmental Science & Technology, 2018, 52, 8501-8509.	10.0	46
15	Hydration mechanisms of Cu2+: tetra-, penta- or hexa-coordinated?. Physical Chemistry Chemical Physics, 2010, 12, 10801.	2.8	45
16	Solution Structures and Acidity Constants of Molybdic Acid. Journal of Physical Chemistry Letters, 2013, 4, 2926-2930.	4.6	39
17	Molecular-level understanding of metal ion retention in clay-rich materials. Nature Reviews Earth & Environment, 2022, 3, 461-476.	29.7	39
18	Acid dissociation mechanisms of Si(OH)4 and Al(H2O)63+ in aqueous solution. Geochimica Et Cosmochimica Acta, 2010, 74, 510-516.	3.9	38

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19	Speciation of gold in hydrosulphide-rich ore-forming fluids: Insights from first-principles molecular dynamics simulations. Geochimica Et Cosmochimica Acta, 2011, 75, 185-194.	3.9	38
20	Surface complexes of acetate on edge surfaces of 2:1 type phyllosilicate: Insights from density functional theory calculation. Geochimica Et Cosmochimica Acta, 2008, 72, 5896-5907.	3.9	34
21	Interfacial structures and acidity of edge surfaces of ferruginous smectites. Geochimica Et Cosmochimica Acta, 2015, 168, 293-301.	3.9	34
22	Silver speciation in chloride-containing hydrothermal solutions from first principles molecular dynamics simulations. Chemical Geology, 2012, 294-295, 103-112.	3.3	33
23	Acidities of confined water in interlayer space of clay minerals. Geochimica Et Cosmochimica Acta, 2011, 75, 4978-4986.	3.9	32
24	Cadmium(II) Complexes Adsorbed on Clay Edge Surfaces: Insight from First Principles Molecular Dynamics Simulation. Clays and Clay Minerals, 2016, 64, 337-347.	1.3	31
25	A combined first principles and classical molecular dynamics study of clay-soil organic matters (SOMs) interactions. Geochimica Et Cosmochimica Acta, 2020, 291, 110-125.	3.9	28
26	Understanding the Heterogeneous Nucleation of Heavy Metal Phyllosilicates on Clay Edges with First-Principles Molecular Dynamics. Environmental Science & Technology, 2019, 53, 13704-13712.	10.0	25
27	Understanding hydration of Zn2+ in hydrothermal fluids with ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2011, 13, 13305.	2.8	24
28	Temperature-Dependent Phase Transition and Desorption Free Energy of Sodium Dodecyl Sulfate at the Water/Vapor Interface: Approaches from Molecular Dynamics Simulations. Langmuir, 2014, 30, 10600-10607.	3.5	24
29	Aqueous Transition-Metal Cations as Impurities in a Wide Gap Oxide: The Cu²⁺/Cu⁺ and Ag²⁺/Ag⁺ Redox Couples Revisited. Journal of Physical Chemistry B, 2015, 119, 1152-1163.	2.6	24
30	Sn(II) chloride speciation and equilibrium Sn isotope fractionation under hydrothermal conditions: A first principles study. Geochimica Et Cosmochimica Acta, 2021, 300, 25-43.	3.9	23
31	Temperature dependence of interfacial structures and acidity of clay edge surfaces. Geochimica Et Cosmochimica Acta, 2015, 160, 91-99.	3.9	22
32	Hydration, acidity and metal complexing of polysulfide species: A first principles molecular dynamics study. Chemical Physics Letters, 2013, 563, 9-14.	2.6	19
33	Distribution and Mobility of Crude Oilâ€“Brine in Clay Mesopores: Insights from Molecular Dynamics Simulations. Langmuir, 2019, 35, 14818-14832.	3.5	19
34	Molecular Dynamics Simulation of the Effects of NaCl on Electrostatic Properties of Newton Black Films. Journal of Physical Chemistry C, 2012, 116, 21913-21922.	3.1	18
35	Specific Counterion Effects on the Atomistic Structure and Capillary-Waves Fluctuation of the Water/Vapor Interface Covered by Sodium Dodecyl Sulfate. Journal of Physical Chemistry C, 2014, 118, 19205-19213.	3.1	18
36	Molecular simulation study on K+â€“Clâ^' ion pair in geological fluids. Acta Geochimica, 2017, 36, 1-8.	1.7	18

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37	An atomic-scale understanding of the initial stage of nucleation of heavy metal cations on clay edges. Geochimica Et Cosmochimica Acta, 2019, 248, 161-171.	3.9	18
38	Complexation of heavy metal cations on clay edges at elevated temperatures. Chemical Geology, 2018, 479, 36-46.	3.3	16
39	First-principles molecular dynamics study of stepwise hydrolysis reactions of Y3+ cations. Chemical Geology, 2012, 334, 37-43.	3.3	15
40	Complexation of carboxylate on smectite surfaces. Physical Chemistry Chemical Physics, 2017, 19, 18400-18406.	2.8	15
41	In Silico Calculation of Acidity Constants of Carbonic Acid Conformers. Journal of Physical Chemistry A, 2010, 114, 12914-12917.	2.5	14
42	First-Principles Molecular Dynamics Insight into Fe²⁺ Complexes Adsorbed on Edge Surfaces of Clay Minerals. Clays and Clay Minerals, 2012, 60, 341-347.	1.3	14
43	Structures and acidity constants of arsenite and thioarsenite species in hydrothermal solutions. Chemical Geology, 2015, 411, 192-199.	3.3	13
44	Introduction to a Special Issue on Molecular Computer Simulations of Clays and Clay-Water Interfaces: Recent Progress, Challenges, and Opportunities. Clays and Clay Minerals, 2016, 64, 335-336.	1.3	13
45	Acidity constants and redox potentials of uranyl ions in hydrothermal solutions. Physical Chemistry Chemical Physics, 2016, 18, 26040-26048.	2.8	13
46	Molecular dynamics simulation of CO₂-switchable surfactant regulated reversible emulsification/demulsification processes of a dodecaneâ€“saline system. Physical Chemistry Chemical Physics, 2020, 22, 23574-23585.	2.8	13
47	Ab Initio Molecular Dynamics Study of Fe-Containing Smectites. Clays and Clay Minerals, 2010, 58, 89-96.	1.3	12
48	A molecular dynamics simulation study of KF and NaF ion pairs in hydrothermal fluids. Fluid Phase Equilibria, 2020, 518, 112625.	2.5	11
49	Surface Acidity and As(V) Complexation of Iron Oxyhydroxides: Insights from First-Principles Molecular Dynamics Simulations. Environmental Science & Technology, 2021, 55, 15921-15928.	10.0	10
50	Molecular Dynamics Simulation of Alkylammonium-Intercalated Vermiculites. Clays and Clay Minerals, 2017, 65, 378-386.	1.3	9
51	Uranyl Arsenate Complexes in Aqueous Solution: Insights from First-Principles Molecular Dynamics Simulations. Inorganic Chemistry, 2018, 57, 5801-5809.	4.0	9
52	Atomistic simulation on mixing thermodynamics of calcite-smithsonite solid solutions. American Mineralogist, 2015, 100, 172-180.	1.9	8
53	Coordination of Zr4+/Hf4+/Nb5+/Ta5+ in silicate melts: insight from first principles molecular dynamics simulations. Chemical Geology, 2020, 555, 119814.	3.3	8
54	Quantum-chemical modelling of clay mineral surfaces and clay mineralâ€“surfaceâ€“adsorbate interactions. Developments in Clay Science, 2018, 9, 49-87.	0.5	7

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55	Interfacial structures and acidity constants of goethite from first-principles Molecular Dynamics simulations. American Mineralogist, 2021, 106, 1736-1743.	1.9	7
56	Structures and Acidity Constants of Silverâ€“Sulfide Complexes in Hydrothermal Fluids: A First-Principles Molecular Dynamics Study. Journal of Physical Chemistry A, 2016, 120, 8435-8443.	2.5	6
57	Complexation of quinone species on 2:1 dioctahedral phyllosilicate surfaces. Applied Clay Science, 2018, 162, 268-275.	5.2	6
58	Mechanism of Base-Promoted Dehydrochlorination of Pentachloroethane: Concerted or Stepwise?. Journal of Physical Chemistry A, 2009, 113, 3542-3544.	2.5	5
59	A molecular dynamics study of Li speciation in hydrothermal fluids and silicate melts. Chemical Geology, 2021, 584, 120528.	3.3	5
60	Redox potentials of aryl derivatives from hybrid functional based first principles molecular dynamics. Physical Chemistry Chemical Physics, 2016, 18, 14911-14917.	2.8	4
61	Adsorption of CTAB on Sapphire-c at High pH: Surface and Zeta Potential Measurements Combined with Sum-Frequency and Second-Harmonic Generation. Langmuir, 2022, 38, 3380-3391.	3.5	4
62	A molecular dynamics study of uranyl-carbonate complexes adsorbed on basal surfaces of clay minerals. Diqiu Huaxue, 2015, 34, 143-155.	0.5	3
63	Frontispiece: Aligning Electronic and Protonic Energy Levels of Protonâ€Coupled Electron Transfer in Water Oxidation on Aqueous TiO₂. Angewandte Chemie - International Edition, 2014, 53, .	13.8	0
64	A molecular simulation study of Cs-Cl and Cs-F ion pairs in hydrothermal fluids. Acta Geochimica, 0, , 1.	1.7	0