

Yun Liu

List of Publications by Year in descending order

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46
papers

1,100
citations

394421

19
h-index

395702

33
g-index

46
all docs

46
docs citations

46
times ranked

1005
citing authors

#	ARTICLE	IF	CITATIONS
1	Ab initio molecular orbital calculations for boron isotope fractionations on boric acids and borates. <i>Geochimica Et Cosmochimica Acta</i> , 2005, 69, 3995-4006.	3.9	150
2	Equilibrium mass-dependent fractionation relationships for triple oxygen isotopes. <i>Geochimica Et Cosmochimica Acta</i> , 2011, 75, 7435-7445.	3.9	109
3	On the proper use of the Bigeleisen-Mayer equation and corrections to it in the calculation of isotopic fractionation equilibrium constants. <i>Geochimica Et Cosmochimica Acta</i> , 2010, 74, 6965-6983.	3.9	81
4	Theoretical prediction for several important equilibrium Ge isotope fractionation factors and geological implications. <i>Earth and Planetary Science Letters</i> , 2009, 287, 1-11.	4.4	72
5	First-principles investigation of vanadium isotope fractionation in solution and during adsorption. <i>Earth and Planetary Science Letters</i> , 2015, 426, 216-224.	4.4	58
6	Equilibrium Se isotope fractionation parameters: A first-principles study. <i>Earth and Planetary Science Letters</i> , 2011, 304, 113-120.	4.4	57
7	Mechanism for the dissolution of olivine series minerals in acidic solutions. <i>American Mineralogist</i> , 2006, 91, 455-458.	1.9	50
8	First-principles study of Ge isotope fractionation during adsorption onto Fe(III)-oxyhydroxide surfaces. <i>Chemical Geology</i> , 2010, 278, 15-22.	3.3	46
9	Theoretical estimation of the equilibrium distribution of clumped isotopes in nature. <i>Geochimica Et Cosmochimica Acta</i> , 2012, 77, 292-303.	3.9	44
10	Theoretical calibration of the triple oxygen isotope thermometer. <i>Geochimica Et Cosmochimica Acta</i> , 2018, 235, 237-245.	3.9	43
11	Equilibrium Mg isotope fractionation among aqueous Mg ²⁺ , carbonates, brucite and lizardite: Insights from first-principles molecular dynamics simulations. <i>Geochimica Et Cosmochimica Acta</i> , 2019, 250, 117-129.	3.9	40
12	Theoretical calculation of equilibrium Mg isotope fractionations between minerals and aqueous solutions. <i>Chemical Geology</i> , 2018, 488, 62-75.	3.3	36
13	Clumped-isotope signatures at equilibrium of CH ₄ , NH ₃ , H ₂ O, H ₂ S and SO ₂ . <i>Geochimica Et Cosmochimica Acta</i> , 2016, 175, 252-270.	3.9	34
14	Molecular-level mechanisms of quartz dissolution under neutral and alkaline conditions in the presence of electrolytes. <i>Geochemical Journal</i> , 2014, 48, 189-205.	1.0	28
15	Nuclear volume effects in equilibrium stable isotope fractionations of mercury, thallium and lead. <i>Scientific Reports</i> , 2015, 5, 12626.	3.3	28
16	A theoretical model of isotopic fractionation by thermal diffusion and its implementation on silicate melts. <i>Geochimica Et Cosmochimica Acta</i> , 2015, 154, 18-27.	3.9	26
17	Equilibrium and kinetic Si isotope fractionation factors and their implications for Si isotope distributions in the Earth's surface environments. <i>Acta Geochimica</i> , 2016, 35, 15-24.	1.7	24
18	Silicon isotope fractionation during the precipitation of quartz and the adsorption of H ₄ SiO ₄ (aq) on Fe(III)-oxyhydroxide surfaces. <i>Diqiu Huaxue</i> , 2015, 34, 459-468.	0.5	23

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19	Nitrogen isotope fractionations among gaseous and aqueous NH ₄ ⁺ , NH ₃ , N ₂ , and metal-ammine complexes: Theoretical calculations and applications. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 295, 80-97.	3.9	21
20	Non-traditional stable isotope behaviors in immiscible silica-melts in a mafic magma chamber. <i>Scientific Reports</i> , 2015, 5, 17561.	3.3	17
21	Nuclear field shift effects on stable isotope fractionation: a review. <i>Acta Geochimica</i> , 2016, 35, 227-239.	1.7	17
22	The theory of equilibrium isotope fractionations for gaseous molecules under super-cold conditions. <i>Geochimica Et Cosmochimica Acta</i> , 2018, 238, 123-149.	3.9	14
23	Predicting equilibrium intramolecular isotope distribution within a large organic molecule by the cutoff calculation. <i>Geochimica Et Cosmochimica Acta</i> , 2020, 269, 292-302.	3.9	11
24	First-principles calculations of equilibrium bromine isotope fractionations. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 297, 65-81.	3.9	10
25	Molecular-Level Mechanism of Phosphoric Acid Digestion of Carbonates and Recalibration of the ¹³ C- ¹⁸ O Clumped Isotope Thermometer. <i>ACS Earth and Space Chemistry</i> , 2020, 4, 420-433.	2.7	9
26	Triple oxygen isotope constraints on the origin of ocean island basalts. <i>Acta Geochimica</i> , 2019, 38, 327-334.	1.7	8
27	Predicting nitrogen and oxygen kinetic isotope effects of nitrate reduction by periplasmic dissimilatory nitrate reductase. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 293, 224-239.	3.9	8
28	Zinc isotope fractionation under vaporization processes and in aqueous solutions. <i>Acta Geochimica</i> , 2018, 37, 663-675.	1.7	7
29	How to produce isotope anomalies in mantle by using extremely small isotope fractionations: A process-driven amplification effect?. <i>Geochimica Et Cosmochimica Acta</i> , 2020, 291, 19-49.	3.9	4
30	Equilibrium thallium isotope fractionation and its constraint on Earth's late veneer. <i>Acta Geochimica</i> , 2019, 38, 459-471.	1.7	3
31	A model of crust-mantle differentiation for the early Earth. <i>Acta Geochimica</i> , 2022, 41, 689-703.	1.7	3
32	Iron-Carbon Alloy Under Shock Compression: Implications for the Carbon Concentration in Earth's Inner Core. <i>Journal of Geophysical Research: Solid Earth</i> , 2022, 127, .	3.4	3
33	Quantum-mechanical equilibrium isotopic fractionation correction to radiocarbon dating: a theory study. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2012, 292, 335-338.	1.5	2
34	Finite Element Method for Modeling 3D Resistivity Sounding on Anisotropic Geoelectric Media. <i>Mathematical Problems in Engineering</i> , 2017, 2017, 1-12.	1.1	2
35	A Metastable Fo-III Wedge in Cold Slabs Subducted to the Lower Part of the Mantle Transition Zone: A Hypothesis Based on First-Principles Simulations. <i>Minerals (Basel, Switzerland)</i> , 2019, 9, 186.	2.0	2
36	Chemical structure of the Earth's mantle defined by fast diffusion elements like helium. <i>Acta Geochimica</i> , 2020, 39, 1-3.	1.7	2

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37	Theoretical calculation of position-specific carbon and hydrogen isotope equilibriums in butane isomers. <i>Chemical Geology</i> , 2021, 561, 120031.	3.3	2
38	Partial Deoxygenation and Dehydration of Ferric Oxyhydroxide in Earth's Subducting Slabs. <i>Geophysical Research Letters</i> , 2021, 48, e2021GL094446.	4.0	2
39	The core-merging giant impact in Earth's accretion history and its implications. <i>Acta Geochimica</i> , 2022, 41, 553-567.	1.7	1
40	The escape mechanisms of the proto-atmosphere on terrestrial planets: "boil-off" escape, hydrodynamic escape and impact erosion. <i>Acta Geochimica</i> , 2022, 41, 592-606.	1.7	1
41	Electrical and thermal conductivity of Earth's core and its thermal evolution: A review. <i>Acta Geochimica</i> , 2022, 41, 665-688.	1.7	1
42	182W anomalies in mantle: a brief review. <i>Acta Geochimica</i> , 0, , 1.	1.7	1
43	The boron isotopic pale-pH indicator: A theoretical re-evaluation. <i>Diqiu Huaxue</i> , 2006, 25, 16-17.	0.5	0
44	Improved Magnetotelluric Zohdy-Oldenburg Direct Inversion. <i>Mathematical Problems in Engineering</i> , 2013, 2013, 1-8.	1.1	0
45	Theoretical calculation of equilibrium Mg isotope fractionation between silicate melt and its vapor. <i>Acta Geochimica</i> , 2018, 37, 655-662.	1.7	0
46	Equilibrium mercury and lead isotope fractionation caused by nuclear volume effects in crystals. <i>Acta Geochimica</i> , 2021, 40, 150-162.	1.7	0