

Marc Blanchard

List of Publications by Year in descending order

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75
papers

2,378
citations

201385

27
h-index

233125

45
g-index

78
all docs

78
docs citations

78
times ranked

2500
citing authors

#	ARTICLE	IF	CITATIONS
1	Iron isotope fractionation between pyrite (FeS ₂), hematite (Fe ₂ O ₃) and siderite (FeCO ₃): A first-principles density functional theory study. <i>Geochimica Et Cosmochimica Acta</i> , 2009, 73, 6565-6578.	1.6	173
2	Arsenic incorporation into FeS ₂ pyrite and its influence on dissolution: A DFT study. <i>Geochimica Et Cosmochimica Acta</i> , 2007, 71, 624-630.	1.6	149
3	Diffusion of Hydrogen in Minerals. <i>Reviews in Mineralogy and Geochemistry</i> , 2006, 62, 291-320.	2.2	98
4	Equilibrium Fractionation of Non-traditional Isotopes: a Molecular Modeling Perspective. <i>Reviews in Mineralogy and Geochemistry</i> , 2017, 82, 27-63.	2.2	71
5	Theoretical infrared spectrum of OH-defects in forsterite. <i>European Journal of Mineralogy</i> , 2011, 23, 285-292.	0.4	69
6	A carbonate-fluoride defect model for carbonate-rich fluorapatite. <i>American Mineralogist</i> , 2013, 98, 1066-1069.	0.9	69
7	Line-broadening effects in the powder infrared spectrum of apatite. <i>Physics and Chemistry of Minerals</i> , 2011, 38, 111-122.	0.3	68
8	Equilibrium zinc isotope fractionation in Zn-bearing minerals from first-principles calculations. <i>Chemical Geology</i> , 2016, 443, 87-96.	1.4	68
9	First-principles calculation of the infrared spectrum of hematite. <i>American Mineralogist</i> , 2008, 93, 1019-1027.	0.9	61
10	Surface modes in the infrared spectrum of hydrous minerals: the OH stretching modes of bayerite. <i>Physics and Chemistry of Minerals</i> , 2008, 35, 279-285.	0.3	55
11	Equilibrium magnesium isotope fractionation between aqueous Mg ²⁺ and carbonate minerals: Insights from path integral molecular dynamics. <i>Geochimica Et Cosmochimica Acta</i> , 2015, 163, 126-139.	1.6	55
12	Theoretical infrared absorption coefficient of OH groups in minerals. <i>American Mineralogist</i> , 2008, 93, 950-953.	0.9	54
13	The nature and partitioning of invisible gold in the pyrite-fluid system. <i>Ore Geology Reviews</i> , 2019, 109, 545-563.	1.1	53
14	First-principles study of boron speciation in calcite and aragonite. <i>Geochimica Et Cosmochimica Acta</i> , 2016, 193, 119-131.	1.6	52
15	Arsenic Incorporation in Pyrite at Ambient Temperature at Both Tetrahedral S ^I and Octahedral Fe ^{II} Sites: Evidence from EXAFS and DFT Analysis. <i>Environmental Science & Technology</i> , 2017, 51, 150-158.	4.6	49
16	Adsorption of As(OH) ₃ on the (001) Surface of FeS ₂ Pyrite: A Quantum-mechanical DFT Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 11390-11396.	1.5	47
17	Incorporation of water in iron-free ringwoodite: A first-principles study. <i>American Mineralogist</i> , 2009, 94, 83-89.	0.9	44
18	Clumped fluoride-hydroxyl defects in forsterite: Implications for the upper-mantle. <i>Earth and Planetary Science Letters</i> , 2014, 390, 287-295.	1.8	42

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19	First-principles simulation of arsenate adsorption on the (111) surface of hematite. <i>Geochimica Et Cosmochimica Acta</i> , 2012, 86, 182-185.	1.6	40
20	First-principles investigation of equilibrium isotopic fractionation of O- and Si-isotopes between refractory solids and gases in the solar nebula. <i>Earth and Planetary Science Letters</i> , 2012, 319-320, 118-127.	1.8	39
21	Strong electric fields at a prototypical oxide/water interface probed by ab initio molecular dynamics: MgO(001). <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 20382-20390.	1.3	39
22	Effect of iron and trivalent cations on OH defects in olivine. <i>American Mineralogist</i> , 2017, 102, 302-311.	0.9	39
23	Reduced partition function ratios of iron and oxygen in goethite. <i>Geochimica Et Cosmochimica Acta</i> , 2015, 151, 19-33.	1.6	38
24	Electronic Structure Study of the High-pressure Vibrational Spectrum of FeS ₂ Pyrite. <i>Journal of Physical Chemistry B</i> , 2005, 109, 22067-22073.	1.2	36
25	Hydrogen diffusion in Dora Maira pyrope. <i>Physics and Chemistry of Minerals</i> , 2004, 31, 593-605.	0.3	33
26	Theoretical isotopic fractionation between structural boron in carbonates and aqueous boric acid and borate ion. <i>Geochimica Et Cosmochimica Acta</i> , 2018, 222, 117-129.	1.6	33
27	First-principles study of the structural and isotopic properties of Al- and OH-bearing hematite. <i>Geochimica Et Cosmochimica Acta</i> , 2010, 74, 3948-3962.	1.6	32
28	An arsenic-driven pump for invisible gold in hydrothermal systems. <i>Geochemical Perspectives Letters</i> , 0, 17, 39-44.	1.0	32
29	Identification of hydrogen defects linked to boron substitution in synthetic forsterite and natural olivine. <i>American Mineralogist</i> , 2014, 99, 2138-2141.	0.9	28
30	First-principles modeling of sulfate incorporation and ³⁴ S/ ³² S isotopic fractionation in different calcium carbonates. <i>Chemical Geology</i> , 2014, 374-375, 84-91.	1.4	26
31	Equilibrium isotopic fractionation between aqueous Zn and minerals from first-principles calculations. <i>Chemical Geology</i> , 2018, 483, 342-350.	1.4	26
32	Experimental and theoretical modelling of kinetic and equilibrium Ba isotope fractionation during calcite and aragonite precipitation. <i>Geochimica Et Cosmochimica Acta</i> , 2020, 269, 566-580.	1.6	26
33	Equilibrium fractionation of H and O isotopes in water from path integral molecular dynamics. <i>Geochimica Et Cosmochimica Acta</i> , 2014, 135, 203-216.	1.6	25
34	Kinetics of hydrogen extraction and deuteration in grossular. <i>Mineralogical Magazine</i> , 2005, 69, 359-371.	0.6	24
35	Infrared spectroscopic properties of goethite: anharmonic broadening, long-range electrostatic effects and Al substitution. <i>Physics and Chemistry of Minerals</i> , 2014, 41, 289-302.	0.3	24
36	Local environment of arsenic in sulfide minerals: insights from high-resolution X-ray spectroscopies, and first-principles calculations at the As K-edge. <i>Journal of Analytical Atomic Spectrometry</i> , 2018, 33, 2070-2082.	1.6	24

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37	Kinetics of deuteration in pyrope. <i>European Journal of Mineralogy</i> , 2004, 16, 567-576.	0.4	23
38	Pressure-induced phase transition in MnCO_3 and its implications on the deep carbon cycle. <i>Journal of Geophysical Research: Solid Earth</i> , 2015, 120, 4069-4079.	1.4	23
39	Experimental and theoretical study of the vibrational properties of diaspore (AlOOH). <i>Physics and Chemistry of Minerals</i> , 2012, 39, 93-102.	0.3	22
40	Comment on "New data on equilibrium iron isotope fractionation among sulfides: Constraints on mechanisms of sulfide formation in hydrothermal and igneous systems" by V.B. Polyakov and D.M. Soutanov. <i>Geochimica Et Cosmochimica Acta</i> , 2012, 87, 356-359.	1.6	21
41	Combination of Inelastic Neutron Scattering Experiments and ab Initio Quantum Calculations for the Study of the Hydration Properties of Oriented Saponites. <i>Journal of Physical Chemistry C</i> , 2017, 121, 5029-5040.	1.5	21
42	First-principles modeling of chlorine isotope fractionation between chloride-bearing molecules and minerals. <i>Chemical Geology</i> , 2019, 525, 424-434.	1.4	21
43	Theoretical investigation of the anomalous equilibrium fractionation of multiple sulfur isotopes during adsorption. <i>Earth and Planetary Science Letters</i> , 2009, 284, 88-93.	1.8	20
44	A computer simulation study of the effect of pressure on Mg diffusion in forsterite. <i>Physics of the Earth and Planetary Interiors</i> , 2009, 172, 13-19.	0.7	20
45	Contribution of interstitial OH groups to the incorporation of water in forsterite. <i>Physics and Chemistry of Minerals</i> , 2014, 41, 105-114.	0.3	20
46	Infrared spectroscopic study of the synthetic Mg-Ni talc series. <i>Physics and Chemistry of Minerals</i> , 2018, 45, 843-854.	0.3	20
47	Clues from ab Initio Calculations on Titanium Isotopic Fractionation in Tholeiitic and Calc-Alkaline Magma Series. <i>ACS Earth and Space Chemistry</i> , 2021, 5, 2466-2480.	1.2	19
48	Structure and theoretical infrared spectra of OH defects in quartz. <i>European Journal of Mineralogy</i> , 2020, 32, 311-323.	0.4	19
49	A computer simulation study of OH defects in Mg_2SiO_4 and Mg_2GeO_4 spinels. <i>Physics and Chemistry of Minerals</i> , 2005, 32, 585-593.	0.3	18
50	Theoretical study of OH-defects in pure enstatite. <i>Physics and Chemistry of Minerals</i> , 2013, 40, 41-50.	0.3	18
51	First-principles calculation of iron and silicon isotope fractionation between Fe-bearing minerals at magmatic temperatures: The importance of second atomic neighbors. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 304, 101-118.	1.6	17
52	Atomistic simulation of Mg_2SiO_4 and Mg_2GeO_4 spinels: a new model. <i>Physics and Chemistry of Minerals</i> , 2005, 32, 332-338.	0.3	16
53	The Extent, Nature, and Origin of K and Rb Depletions and Isotopic Fractionations in Earth, the Moon, and Other Planetary Bodies. <i>Planetary Science Journal</i> , 2022, 3, 29.	1.5	16
54	Probing the local environment of substitutional Al^{3+} in goethite using X-ray absorption spectroscopy and first-principles calculations. <i>Physics and Chemistry of Minerals</i> , 2016, 43, 217-227.	0.3	15

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55	Theoretical Raman spectrum and anharmonicity of tetrahedral OH defects in hydrous forsterite. <i>European Journal of Mineralogy</i> , 2017, 29, 201-212.	0.4	15
56	New constraints on Xe incorporation mechanisms in olivine from first-principles calculations. <i>Geochimica Et Cosmochimica Acta</i> , 2018, 222, 146-155.	1.6	14
57	Infrared signatures of OH-defects in wadsleyite: A first-principles study. <i>American Mineralogist</i> , 2013, 98, 2132-2143.	0.9	13
58	Theoretical infrared spectrum of partially protonated cationic vacancies in forsterite. <i>European Journal of Mineralogy</i> , 2014, 26, 203-210.	0.4	13
59	Infrared spectroscopic study of sulfate-bearing calcite from deep-sea bamboo coral. <i>European Journal of Mineralogy</i> , 2017, 29, 397-408.	0.4	13
60	Site-specific equilibrium isotopic fractionation of oxygen, carbon and calcium in apatite. <i>Geochimica Et Cosmochimica Acta</i> , 2017, 219, 57-73.	1.6	13
61	Spectroscopic investigation and theoretical modeling of kaolinite-group minerals and other low-temperature phases. <i>Comptes Rendus - Geoscience</i> , 2011, 343, 177-187.	0.4	12
62	First-principles study of OH defects in zircon. <i>Physics and Chemistry of Minerals</i> , 2013, 40, 547-554.	0.3	12
63	Theoretical study of the local charge compensation and spectroscopic properties of B-type carbonate defects in apatite. <i>Physics and Chemistry of Minerals</i> , 2014, 41, 347-359.	0.3	11
64	Job submission to grid computing environments. <i>Concurrency Computation Practice and Experience</i> , 2008, 20, 1329-1340.	1.4	10
65	van der Waals Contribution to the Relative Stability of Aqueous Zn(2+) Coordination States. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3340-3347.	2.3	10
66	Influence of trace level As or Ni on pyrite formation kinetics at low temperature. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 300, 333-353.	1.6	9
67	First-principles investigation of equilibrium iron isotope fractionation in Fe1â ¹ S alloys at Earth's core formation conditions. <i>Earth and Planetary Science Letters</i> , 2021, 569, 117059.	1.8	8
68	The Xeâ€SiO 2 System at Moderate Pressure and High Temperature. <i>Geochemistry, Geophysics, Geosystems</i> , 2019, 20, 992-1003.	1.0	7
69	Mechanisms and rates of pyrite formation from hydrothermal fluid revealed by iron isotopes. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 304, 281-304.	1.6	7
70	A stable isotope toolbox for water and inorganic carbon cycle studies. <i>Nature Reviews Earth & Environment</i> , 2021, 2, 699-719.	12.2	7
71	Kr environment in feldspathic glass and melt: A high pressure, high temperature X-ray absorption study. <i>Chemical Geology</i> , 2018, 493, 525-531.	1.4	6
72	First-principles modeling of X-ray absorption spectra enlightens the processes of scandium sequestration by iron oxides. <i>American Mineralogist</i> , 2020, 105, 1099-1103.	0.9	4

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73	2 Equilibrium Fractionation of Non-traditional Isotopes: a Molecular Modeling Perspective. , 2017, , .		2
74	Electronic Structure Study of the High-Pressure Vibrational Spectrum of FeS ₂ Pyrite.. ChemInform, 2006, 37, no.	0.1	0
75	Melt Percolation, Concentration and Dyking in the Hawaiian Mantle Plume and Overriding Lithosphere: Links to the Evolution of Lava Composition along the Volcanic Chain. Journal of Petrology, 2022, 63, .	1.1	0