Marc Blanchard

List of Publications by Year
in descending order

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75 papers	2,378 citations	201674 27 h-index	233421 45 g-index
78 all docs	78 docs citations	78 times ranked	2500 citing authors

#	Article	IF	Citations
1	Iron isotope fractionation between pyrite (FeS2), hematite (Fe2O3) and siderite (FeCO3): A first-principles density functional theory study. Geochimica Et Cosmochimica Acta, 2009, 73, 6565-6578.	3.9	173
2	Arsenic incorporation into FeS2 pyrite and its influence on dissolution: A DFT study. Geochimica Et Cosmochimica Acta, 2007, 71, 624-630.	3.9	149
3	Diffusion of Hydrogen in Minerals. Reviews in Mineralogy and Geochemistry, 2006, 62, 291-320.	4.8	98
4	Equilibrium Fractionation of Non-traditional Isotopes: a Molecular Modeling Perspective. Reviews in Mineralogy and Geochemistry, 2017, 82, 27-63.	4.8	71
5	Theoretical infrared spectrum of OH-defects in forsterite. European Journal of Mineralogy, 2011, 23, 285-292.	1.3	69
6	A carbonate-fluoride defect model for carbonate-rich fluorapatite. American Mineralogist, 2013, 98, 1066-1069.	1.9	69
7	Line-broadening effects in the powder infrared spectrum of apatite. Physics and Chemistry of Minerals, 2011, 38, 111-122.	0.8	68
8	Equilibrium zinc isotope fractionation in Zn-bearing minerals from first-principlesÂcalculations. Chemical Geology, 2016, 443, 87-96.	3.3	68
9	First-principles calculation of the infrared spectrum of hematite. American Mineralogist, 2008, 93, 1019-1027.	1.9	61
10	Surface modes in the infrared spectrum of hydrous minerals: the OH stretching modes of bayerite. Physics and Chemistry of Minerals, 2008, 35, 279-285.	0.8	55
11	Equilibrium magnesium isotope fractionation between aqueous Mg2+ and carbonate minerals: Insights from path integral molecular dynamics. Geochimica Et Cosmochimica Acta, 2015, 163, 126-139.	3.9	55
12	Theoretical infrared absorption coefficient of OH groups in minerals. American Mineralogist, 2008, 93, 950-953.	1.9	54
13	The nature and partitioning of invisible gold in the pyrite-fluid system. Ore Geology Reviews, 2019, 109, 545-563.	2.7	53
14	First-principles study of boron speciation in calcite and aragonite. Geochimica Et Cosmochimica Acta, 2016, 193, 119-131.	3.9	52
15	Arsenic Incorporation in Pyrite at Ambient Temperature at Both Tetrahedral S^{â€“I} and Octahedral Fe^{II} Sites: Evidence from EXAFSâ€“DFT Analysis. Environmental Science & Technology, 2017, 51, 150-158.	10.0	49
16	Adsorption of As(OH)₃ on the (001) Surface of FeS₂ Pyrite:â€‰ A Quantum-mechanical DFT Study. Journal of Physical Chemistry C, 2007, 111, 11390-11396.	3.1	47
17	Incorporation of water in iron-free ringwoodite: A first-principles study. American Mineralogist, 2009, 94, 83-89.	1.9	44
18	Clumped fluoride-hydroxyl defects in forsterite: Implications for the upper-mantle. Earth and Planetary Science Letters, 2014, 390, 287-295.	4.4	42

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19	First-principles simulation of arsenate adsorption on the (1<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 757 Td (xmlns:mm surface of hematite. Geochimica Et Cosmochimica Acta, 2012, 86, 182-195.	3.9	40
20	First-principles investigation of equilibrium isotopic fractionation of O- and Si-isotopes between refractory solids and gases in the solar nebula. Earth and Planetary Science Letters, 2012, 319-320, 118-127.	4.4	39
21	Strong electric fields at a prototypical oxide/water interface probed by ab initio molecular dynamics: MgO(001). Physical Chemistry Chemical Physics, 2015, 17, 20382-20390.	2.8	39
22	Effect of iron and trivalent cations on OH defects in olivine. American Mineralogist, 2017, 102, 302-311.	1.9	39
23	Reduced partition function ratios of iron and oxygen in goethite. Geochimica Et Cosmochimica Acta, 2015, 151, 19-33.	3.9	38
24	Electronic Structure Study of the High-pressure Vibrational Spectrum of FeS2Pyrite. Journal of Physical Chemistry B, 2005, 109, 22067-22073.	2.6	36
25	Hydrogen diffusion in Dora Maira pyrope. Physics and Chemistry of Minerals, 2004, 31, 593-605.	0.8	33
26	Theoretical isotopic fractionation between structural boron in carbonates and aqueous boric acid and borate ion. Geochimica Et Cosmochimica Acta, 2018, 222, 117-129.	3.9	33
27	First-principles study of the structural and isotopic properties of Al- and OH-bearing hematite. Geochimica Et Cosmochimica Acta, 2010, 74, 3948-3962.	3.9	32
28	An arsenic-driven pump for invisible gold in hydrothermal systems. Geochemical Perspectives Letters, 0, 17, 39-44.	5.0	32
29	Identification of hydrogen defects linked to boron substitution in synthetic forsterite and natural olivine. American Mineralogist, 2014, 99, 2138-2141.	1.9	28
30	First-principles modeling of sulfate incorporation and 34S/32S isotopic fractionation in different calcium carbonates. Chemical Geology, 2014, 374-375, 84-91.	3.3	26
31	Equilibrium isotopic fractionation between aqueous Zn and minerals from first-principles calculations. Chemical Geology, 2018, 483, 342-350.	3.3	26
32	Experimental and theoretical modelling of kinetic and equilibrium Ba isotope fractionation during calcite and aragonite precipitation. Geochimica Et Cosmochimica Acta, 2020, 269, 566-580.	3.9	26
33	Equilibrium fractionation of H and O isotopes in water from path integral molecular dynamics. Geochimica Et Cosmochimica Acta, 2014, 135, 203-216.	3.9	25
34	Kinetics of hydrogen extraction and deuteration in grossular. Mineralogical Magazine, 2005, 69, 359-371.	1.4	24
35	Infrared spectroscopic properties of goethite: anharmonic broadening, long-range electrostatic effects and Al substitution. Physics and Chemistry of Minerals, 2014, 41, 289-302.	0.8	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. Journal of Analytical Atomic Spectrometry, 2018, 33, 2070-2082.	3.0	24

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37	Kinetics of deuteration in pyrope. European Journal of Mineralogy, 2004, 16, 567-576.	1.3	23
38	Pressureâ€•induced phase transition in MnCO₃ and its implications on the deep carbon cycle. Journal of Geophysical Research: Solid Earth, 2015, 120, 4069-4079.	3.4	23
39	Experimental and theoretical study of the vibrational properties of diaspore (Î±-AlOOH). Physics and Chemistry of Minerals, 2012, 39, 93-102.	0.8	22
40	Comment on â€œNew data on equilibrium iron isotope fractionation among sulfides: Constraints on mechanisms of sulfide formation in hydrothermal and igneous systemsâ€•by V.B. Polyakov and D.M. Soultanov. Geochimica Et Cosmochimica Acta, 2012, 87, 356-359.	3.9	21
41	Combination of Inelastic Neutron Scattering Experiments and ab Initio Quantum Calculations for the Study of the Hydration Properties of Oriented Saponites. Journal of Physical Chemistry C, 2017, 121, 5029-5040.	3.1	21
42	First-principles modeling of chlorine isotope fractionation between chloride-bearing molecules and minerals. Chemical Geology, 2019, 525, 424-434.	3.3	21
43	Theoretical investigation of the anomalous equilibrium fractionation of multiple sulfur isotopes during adsorption. Earth and Planetary Science Letters, 2009, 284, 88-93.	4.4	20
44	A computer simulation study of the effect of pressure on Mg diffusion in forsterite. Physics of the Earth and Planetary Interiors, 2009, 172, 13-19.	1.9	20
45	Contribution of interstitial OH groups to the incorporation of water in forsterite. Physics and Chemistry of Minerals, 2014, 41, 105-114.	0.8	20
46	Infrared spectroscopic study of the synthetic Mgâ€“Ni talc series. Physics and Chemistry of Minerals, 2018, 45, 843-854.	0.8	20
47	Clues from Ab Initio Calculations on Titanium Isotopic Fractionation in Tholeiitic and Calc-Alkaline Magma Series. ACS Earth and Space Chemistry, 2021, 5, 2466-2480.	2.7	19
48	Structure and theoretical infrared spectra of OH defects in quartz. European Journal of Mineralogy, 2020, 32, 311-323.	1.3	19
49	A computer simulation study of OH defects in Mg2SiO4 and Mg2GeO4 spinels. Physics and Chemistry of Minerals, 2005, 32, 585-593.	0.8	18
50	Theoretical study of OH-defects in pure enstatite. Physics and Chemistry of Minerals, 2013, 40, 41-50.	0.8	18
51	First-principles calculation of iron and silicon isotope fractionation between Fe-bearing minerals at magmatic temperatures: The importance of second atomic neighbors. Geochimica Et Cosmochimica Acta, 2021, 304, 101-118.	3.9	17
52	Atomistic simulation of Mg2SiO4 and Mg2GeO4 spinels: a new model. Physics and Chemistry of Minerals, 2005, 32, 332-338.	0.8	16
53	The Extent, Nature, and Origin of K and Rb Depletions and Isotopic Fractionations in Earth, the Moon, and Other Planetary Bodies. Planetary Science Journal, 2022, 3, 29.	3.6	16
54	Probing the local environment of substitutional Al $$^{3+}$$ 3 + in goethite using X-ray absorption spectroscopy and first-principles calculations. Physics and Chemistry of Minerals, 2016, 43, 217-227.	0.8	15

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55	Theoretical Raman spectrum and anharmonicity of tetrahedral OH defects in hydrous forsterite. European Journal of Mineralogy, 2017, 29, 201-212.	1.3	15
56	New constraints on Xe incorporation mechanisms in olivine from first-principles calculations. Geochimica Et Cosmochimica Acta, 2018, 222, 146-155.	3.9	14
57	Infrared signatures of OH-defects in wadsleyite: A first-principles study. American Mineralogist, 2013, 98, 2132-2143.	1.9	13
58	Theoretical infrared spectrum of partially protonated cationic vacancies in forsterite. European Journal of Mineralogy, 2014, 26, 203-210.	1.3	13
59	Infrared spectroscopic study of sulfate-bearing calcite from deep-sea bamboo coral. European Journal of Mineralogy, 2017, 29, 397-408.	1.3	13
60	Site-specific equilibrium isotopic fractionation of oxygen, carbon and calcium in apatite. Geochimica Et Cosmochimica Acta, 2017, 219, 57-73.	3.9	13
61	Spectroscopic investigation and theoretical modeling of kaolinite-group minerals and other low-temperature phases. Comptes Rendus - Geoscience, 2011, 343, 177-187.	1.2	12
62	First-principles study of OH defects in zircon. Physics and Chemistry of Minerals, 2013, 40, 547-554.	0.8	12
63	Theoretical study of the local charge compensation and spectroscopic properties of B-type carbonate defects in apatite. Physics and Chemistry of Minerals, 2014, 41, 347-359.	0.8	11
64	Job submission to grid computing environments. Concurrency Computation Practice and Experience, 2008, 20, 1329-1340.	2.2	10
65	van der Waals Contribution to the Relative Stability of Aqueous Zn(2+) Coordination States. Journal of Chemical Theory and Computation, 2017, 13, 3340-3347.	5.3	10
66	Influence of trace level As or Ni on pyrite formation kinetics at low temperature. Geochimica Et Cosmochimica Acta, 2021, 300, 333-353.	3.9	9
67	First-principles investigation of equilibrium iron isotope fractionation in Fe1â”'S alloys at Earth's core formation conditions. Earth and Planetary Science Letters, 2021, 569, 117059.	4.4	8
68	The Xeâ€šiO 2 System at Moderate Pressure and High Temperature. Geochemistry, Geophysics, Geosystems, 2019, 20, 992-1003.	2.5	7
69	Mechanisms and rates of pyrite formation from hydrothermal fluid revealed by iron isotopes. Geochimica Et Cosmochimica Acta, 2021, 304, 281-304.	3.9	7
70	A stable isotope toolbox for water and inorganic carbon cycle studies. Nature Reviews Earth & Environment, 2021, 2, 699-719.	29.7	7
71	Kr environment in feldspathic glass and melt: A high pressure, high temperature X-ray absorption study. Chemical Geology, 2018, 493, 525-531.	3.3	6
72	First-principles modeling of X-ray absorption spectra enlightens the processes of scandium sequestration by iron oxides. American Mineralogist, 2020, 105, 1099-1103.	1.9	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 FeS2 Pyrite.. ChemInform, 2006, 37, no.	0.0	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, .	2.8	0