

# 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	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.	3.6	16
2	Melt Percolation, Concentration and Dyking in the Hawaiian Mantle Plume and Overriding Lithosphere: Links to the Evolution of Lava Composition along the Volcanic Chain. <i>Journal of Petrology</i> , 2022, 63, .	2.8	0
3	Influence of trace level As or Ni on pyrite formation kinetics at low temperature. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 300, 333-353.	3.9	9
4	Mechanisms and rates of pyrite formation from hydrothermal fluid revealed by iron isotopes. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 304, 281-304.	3.9	7
5	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.	3.9	17
6	Clues from <i>Ab Initio</i> Calculations on Titanium Isotopic Fractionation in Tholeiitic and Calc-Alkaline Magma Series. <i>ACS Earth and Space Chemistry</i> , 2021, 5, 2466-2480.	2.7	19
7	A stable isotope toolbox for water and inorganic carbon cycle studies. <i>Nature Reviews Earth &amp; Environment</i> , 2021, 2, 699-719.	29.7	7
8	First-principles investigation of equilibrium iron isotope fractionation in Fe <sup>1</sup> S alloys at Earth's core formation conditions. <i>Earth and Planetary Science Letters</i> , 2021, 569, 117059.	4.4	8
9	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.	3.9	26
10	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.	1.9	4
11	Structure and theoretical infrared spectra of OH defects in quartz. <i>European Journal of Mineralogy</i> , 2020, 32, 311-323.	1.3	19
12	First-principles modeling of chlorine isotope fractionation between chloride-bearing molecules and minerals. <i>Chemical Geology</i> , 2019, 525, 424-434.	3.3	21
13	The Xe-SiO <sub>2</sub> System at Moderate Pressure and High Temperature. <i>Geochemistry, Geophysics, Geosystems</i> , 2019, 20, 992-1003.	2.5	7
14	The nature and partitioning of invisible gold in the pyrite-fluid system. <i>Ore Geology Reviews</i> , 2019, 109, 545-563.	2.7	53
15	Equilibrium isotopic fractionation between aqueous Zn and minerals from first-principles calculations. <i>Chemical Geology</i> , 2018, 483, 342-350.	3.3	26
16	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.	3.9	33
17	New constraints on Xe incorporation mechanisms in olivine from first-principles calculations. <i>Geochimica Et Cosmochimica Acta</i> , 2018, 222, 146-155.	3.9	14
18	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.	3.0	24

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19	Infrared spectroscopic study of the synthetic Mg-Ni talc series. <i>Physics and Chemistry of Minerals</i> , 2018, 45, 843-854.	0.8	20
20	Kr environment in feldspathic glass and melt: A high pressure, high temperature X-ray absorption study. <i>Chemical Geology</i> , 2018, 493, 525-531.	3.3	6
21	Equilibrium Fractionation of Non-traditional Isotopes: a Molecular Modeling Perspective. <i>Reviews in Mineralogy and Geochemistry</i> , 2017, 82, 27-63.	4.8	71
22	Effect of iron and trivalent cations on OH defects in olivine. <i>American Mineralogist</i> , 2017, 102, 302-311.	1.9	39
23	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.	3.1	21
24	Theoretical Raman spectrum and anharmonicity of tetrahedral OH defects in hydrous forsterite. <i>European Journal of Mineralogy</i> , 2017, 29, 201-212.	1.3	15
25	Infrared spectroscopic study of sulfate-bearing calcite from deep-sea bamboo coral. <i>European Journal of Mineralogy</i> , 2017, 29, 397-408.	1.3	13
26	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.	5.3	10
27	Site-specific equilibrium isotopic fractionation of oxygen, carbon and calcium in apatite. <i>Geochimica Et Cosmochimica Acta</i> , 2017, 219, 57-73.	3.9	13
28	Arsenic Incorporation in Pyrite at Ambient Temperature at Both Tetrahedral S <sup>IV</sup> and Octahedral Fe <sup>II</sup> Sites: Evidence from EXAFS-DFT Analysis. <i>Environmental Science &amp; Technology</i> , 2017, 51, 150-158.	10.0	49
29	2 Equilibrium Fractionation of Non-traditional Isotopes: a Molecular Modeling Perspective. , 2017, , .		2
30	First-principles study of boron speciation in calcite and aragonite. <i>Geochimica Et Cosmochimica Acta</i> , 2016, 193, 119-131.	3.9	52
31	Equilibrium zinc isotope fractionation in Zn-bearing minerals from first-principles calculations. <i>Chemical Geology</i> , 2016, 443, 87-96.	3.3	68
32	Probing the local environment of substitutional Al <sup>3+</sup> in goethite using X-ray absorption spectroscopy and first-principles calculations. <i>Physics and Chemistry of Minerals</i> , 2016, 43, 217-227.	0.8	15
33	Pressure-induced phase transition in MnCO <sub>3</sub> and its implications on the deep carbon cycle. <i>Journal of Geophysical Research: Solid Earth</i> , 2015, 120, 4069-4079.	3.4	23
34	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.	2.8	39
35	Equilibrium magnesium isotope fractionation between aqueous Mg <sup>2+</sup> and carbonate minerals: Insights from path integral molecular dynamics. <i>Geochimica Et Cosmochimica Acta</i> , 2015, 163, 126-139.	3.9	55
36	Reduced partition function ratios of iron and oxygen in goethite. <i>Geochimica Et Cosmochimica Acta</i> , 2015, 151, 19-33.	3.9	38

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37	Identification of hydrogen defects linked to boron substitution in synthetic forsterite and natural olivine. <i>American Mineralogist</i> , 2014, 99, 2138-2141.	1.9	28
38	Equilibrium fractionation of H and O isotopes in water from path integral molecular dynamics. <i>Geochimica Et Cosmochimica Acta</i> , 2014, 135, 203-216.	3.9	25
39	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.	0.8	11
40	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.	0.8	24
41	Contribution of interstitial OH groups to the incorporation of water in forsterite. <i>Physics and Chemistry of Minerals</i> , 2014, 41, 105-114.	0.8	20
42	First-principles modeling of sulfate incorporation and <sup>34</sup> S/ <sup>32</sup> S isotopic fractionation in different calcium carbonates. <i>Chemical Geology</i> , 2014, 374-375, 84-91.	3.3	26
43	Clumped fluoride-hydroxyl defects in forsterite: Implications for the upper-mantle. <i>Earth and Planetary Science Letters</i> , 2014, 390, 287-295.	4.4	42
44	Theoretical infrared spectrum of partially protonated cationic vacancies in forsterite. <i>European Journal of Mineralogy</i> , 2014, 26, 203-210.	1.3	13
45	First-principles study of OH defects in zircon. <i>Physics and Chemistry of Minerals</i> , 2013, 40, 547-554.	0.8	12
46	Theoretical study of OH-defects in pure enstatite. <i>Physics and Chemistry of Minerals</i> , 2013, 40, 41-50.	0.8	18
47	Infrared signatures of OH-defects in wadsleyite: A first-principles study. <i>American Mineralogist</i> , 2013, 98, 2132-2143.	1.9	13
48	A carbonate-fluoride defect model for carbonate-rich fluorapatite. <i>American Mineralogist</i> , 2013, 98, 1066-1069.	1.9	69
49	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.	4.4	39
50	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.	3.9	21
51	First-principles simulation of arsenate adsorption on the (111) surface of hematite. <i>Geochimica Et Cosmochimica Acta</i> , 2012, 86, 182-195.	3.9	40
52	Experimental and theoretical study of the vibrational properties of diaspore ( $\pm$ -AlOOH). <i>Physics and Chemistry of Minerals</i> , 2012, 39, 93-102.	0.8	22
53	Spectroscopic investigation and theoretical modeling of kaolinite-group minerals and other low-temperature phases. <i>Comptes Rendus - Geoscience</i> , 2011, 343, 177-187.	1.2	12
54	Line-broadening effects in the powder infrared spectrum of apatite. <i>Physics and Chemistry of Minerals</i> , 2011, 38, 111-122.	0.8	68

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55	Theoretical infrared spectrum of OH-defects in forsterite. <i>European Journal of Mineralogy</i> , 2011, 23, 285-292.	1.3	69
56	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.	3.9	32
57	Incorporation of water in iron-free ringwoodite: A first-principles study. <i>American Mineralogist</i> , 2009, 94, 83-89.	1.9	44
58	Theoretical investigation of the anomalous equilibrium fractionation of multiple sulfur isotopes during adsorption. <i>Earth and Planetary Science Letters</i> , 2009, 284, 88-93.	4.4	20
59	Iron isotope fractionation between pyrite (FeS <sub>2</sub> ), hematite (Fe <sub>2</sub> O <sub>3</sub> ) and siderite (FeCO <sub>3</sub> ): A first-principles density functional theory study. <i>Geochimica Et Cosmochimica Acta</i> , 2009, 73, 6565-6578.	3.9	173
60	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.	1.9	20
61	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.	0.8	55
62	Job submission to grid computing environments. <i>Concurrency Computation Practice and Experience</i> , 2008, 20, 1329-1340.	2.2	10
63	Theoretical infrared absorption coefficient of OH groups in minerals. <i>American Mineralogist</i> , 2008, 93, 950-953.	1.9	54
64	First-principles calculation of the infrared spectrum of hematite. <i>American Mineralogist</i> , 2008, 93, 1019-1027.	1.9	61
65	Arsenic incorporation into FeS <sub>2</sub> pyrite and its influence on dissolution: A DFT study. <i>Geochimica Et Cosmochimica Acta</i> , 2007, 71, 624-630.	3.9	149
66	Adsorption of As(OH) <sub>3</sub> on the (001) Surface of FeS <sub>2</sub> Pyrite: A Quantum-mechanical DFT Study. <i>Journal of Physical Chemistry C</i> , 2007, 111, 11390-11396.	3.1	47
67	Diffusion of Hydrogen in Minerals. <i>Reviews in Mineralogy and Geochemistry</i> , 2006, 62, 291-320.	4.8	98
68	Electronic Structure Study of the High-Pressure Vibrational Spectrum of FeS <sub>2</sub> Pyrite.. <i>ChemInform</i> , 2006, 37, no.	0.0	0
69	Atomistic simulation of Mg <sub>2</sub> SiO <sub>4</sub> and Mg <sub>2</sub> GeO <sub>4</sub> spinels: a new model. <i>Physics and Chemistry of Minerals</i> , 2005, 32, 332-338.	0.8	16
70	A computer simulation study of OH defects in Mg <sub>2</sub> SiO <sub>4</sub> and Mg <sub>2</sub> GeO <sub>4</sub> spinels. <i>Physics and Chemistry of Minerals</i> , 2005, 32, 585-593.	0.8	18
71	Kinetics of hydrogen extraction and deuteration in grossular. <i>Mineralogical Magazine</i> , 2005, 69, 359-371.	1.4	24
72	Electronic Structure Study of the High-pressure Vibrational Spectrum of FeS <sub>2</sub> Pyrite. <i>Journal of Physical Chemistry B</i> , 2005, 109, 22067-22073.	2.6	36

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73	Hydrogen diffusion in Dora Maira pyrope. <i>Physics and Chemistry of Minerals</i> , 2004, 31, 593-605.	0.8	33
74	Kinetics of deuteration in pyrope. <i>European Journal of Mineralogy</i> , 2004, 16, 567-576.	1.3	23
75	An arsenic-driven pump for invisible gold in hydrothermal systems. <i>Geochemical Perspectives Letters</i> , 0, 17, 39-44.	5.0	32