Sandro Jahn

List of Publications by Year
in descending order

96 papers	2,401 citations	159585 30 h-index	233421 45 g-index
101 all docs	101 docs citations	101 times ranked	2172 citing authors

#	Article	IF	Citations
1	Microscopic structure of water at elevated pressures and temperatures. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6301-6306.	7.1	127
2	Including many-body effects in models for ionic liquids. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	117
3	Beyond sixfold coordinated Si in SiO ₂ glass at ultrahigh pressures. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10041-10046.	7.1	88
4	Ab initio prediction of equilibrium boron isotope fractionation between minerals and aqueous fluids at high P and T. Geochimica Et Cosmochimica Acta, 2013, 101, 285-301.	3.9	87
5	Multipoles and interaction potentials in ionic materials from planewave-DFT calculations. Faraday Discussions, 2003, 124, 171.	3.2	85
6	Prediction of equilibrium Li isotope fractionation between minerals and aqueous solutions at high P and T: An efficient ab initio approach. Geochimica Et Cosmochimica Acta, 2011, 75, 6112-6123.	3.9	78
7	From first-principles to material properties. Computational and Theoretical Chemistry, 2006, 771, 9-18.	1.5	75
8	Modeling Earth materials from crustal to lower mantle conditions: A transferable set of interaction potentials for the CMAS system. Physics of the Earth and Planetary Interiors, 2007, 162, 129-139.	1.9	75
9	Thermal conductivity of MgO, MgSiO3 perovskite and post-perovskite in the Earth's deep mantle. Earth and Planetary Science Letters, 2012, 355-356, 102-108.	4.4	67
10	Cr(III) solubility in aqueous fluids at high pressures and temperatures. Geochimica Et Cosmochimica Acta, 2014, 126, 212-227.	3.9	65
11	Li-isotope fractionation between silicates and fluids: Pressure dependence and influence of the bonding environment. European Journal of Mineralogy, 2011, 23, 333-342.	1.3	59
12	Lithium speciation in aqueous fluids at high P and T studied by ab initio molecular dynamics and consequences for Li-isotope fractionation between minerals and fluids. Geochimica Et Cosmochimica Acta, 2009, 73, 5428-5434.	3.9	53
13	Structural Transformations on Vitrification in the Fragile Glass-Forming System<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CaAl</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 109, 235501.	7.8	53
14	Mg2SiO4 liquid under high pressure from molecular dynamics. Chemical Geology, 2008, 256, 185-192.	3.3	51
15	Vibrational mode frequencies of silica species in SiO2-H2O liquids and glasses from ab initio molecular dynamics. Journal of Chemical Physics, 2012, 136, 154501.	3.0	50
16	Phase transitions and equation of state of forsterite to 90 GPa from single-crystal X-ray diffraction and molecular modeling. American Mineralogist, 2014, 99, 35-43.	1.9	50
17	Speciation in Aqueous MgSO₄ Fluids at High Pressures and High Temperatures from ab Initio Molecular Dynamics and Raman Spectroscopy. Journal of Physical Chemistry B, 2010, 114, 15565-15572.	2.6	46
18	Condensed phase ionic polarizabilities from plane wave density functional theory calculations. Journal of Chemical Physics, 2006, 125, 144104.	3.0	42

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19	Development of chemical and topological structure in aluminosilicate liquids and glasses at high pressure. Journal of Physics Condensed Matter, 2015, 27, 105103.	1.8	42
20	The structure of liquid calcium aluminates as investigated using neutron and high energy x-ray diffraction in combination with molecular dynamics simulation methods. Journal of Physics Condensed Matter, 2011, 23, 155101.	1.8	41
21	Theoretical Approaches to Structure and Spectroscopy of Earth Materials. Reviews in Mineralogy and Geochemistry, 2014, 78, 691-743.	4.8	41
22	Structure and dynamics in liquid alumina: Simulations with an ab initio interaction potential. Journal of Non-Crystalline Solids, 2007, 353, 3500-3504.	3.1	40
23	Transport properties of Mg2SiO4 liquid at high pressure: Physical state of a magma ocean. Earth and Planetary Science Letters, 2011, 312, 463-470.	4.4	39
24	Shock-induced transformation of olivine to a new metastable (Mg,Fe)2SiO4 polymorph in Martian meteorites. Earth and Planetary Science Letters, 2007, 261, 469-475.	4.4	36
25	Phase transitions in the system CaCO3 at high P and T determined by in situ vibrational spectroscopy in diamond anvil cells and first-principles simulations. Physics and Chemistry of Minerals, 2016, 43, 545-561.	0.8	36
26	Vibrational properties of silica species in MgOâ€“SiO2 glasses obtained from ab initio molecular dynamics. Chemical Geology, 2013, 346, 22-33.	3.3	35
27	Ti K-edge XANES study on the coordination number and oxidation state of Titanium in pyroxene, olivine, armalcolite, ilmenite, and silicate glass during mare basalt petrogenesis. Contributions To Mineralogy and Petrology, 2018, 173, 1.	3.1	35
28	Structure of Normal and Supercooled Liquid Aluminum Oxide. Chemistry of Materials, 2005, 17, 2662-2666.	6.7	34
29	The development of the BRISP spectrometer at the Institut Laue-Langevin. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2005, 544, 620-642.	1.6	32
30	Transferable interaction model forAl2O3. Physical Review B, 2006, 74, .	3.2	32
31	The construction and application of a fully flexible computer simulation model for lithium oxide. Journal of Physics Condensed Matter, 2004, 16, S2795-S2810.	1.8	29
32	Atomic structures and energies of grain boundaries in Mg2SiO4 forsterite from atomistic modeling. Physics and Chemistry of Minerals, 2012, 39, 749-760.	0.8	28
33	High-pressure phase transitions in MgSiO3 orthoenstatite studied by atomistic computer simulation. American Mineralogist, 2008, 93, 528-532.	1.9	27
34	Combined high-pressure and high-temperature vibrational studies of dolomite: phase diagram and evidence of a new distorted modification. Physics and Chemistry of Minerals, 2017, 44, 465-476.	0.8	26
35	Raman spectroscopy of siderite at high pressure: Evidence for a sharp spin transition. American Mineralogist, 2016, 101, 2638-2644.	1.9	22
36	Dynamic simulation of pressure-driven phase transformations in crystalline Al2O3. Physical Review B, 2004, 69, .	3.2	20

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37	The 3.65 A phase, MgSi(OH)6: Structural insights from DFT-calculations and T-dependent IR spectroscopy. American Mineralogist, 2012, 97, 1043-1048.	1.9	19
38	Molecular dynamics simulations of Y in silicate melts and implications for trace element partitioning. Chemical Geology, 2013, 346, 14-21.	3.3	19
39	Plastic deformation of orthoenstatite and the ortho- to high-pressure clinoenstatite transition: a metadynamics simulation study. Physics and Chemistry of Minerals, 2008, 35, 17-23.	0.8	18
40	Equation of state and elasticity of the 3.65 Ã... phase: Implications for the X-discontinuity. American Mineralogist, 2015, 100, 2199-2208.	1.9	17
41	Short- and intermediate-range order in levitated liquid aluminates. Journal of Physics Condensed Matter, 2007, 19, 455210.	1.8	16
42	Vibrational mode frequencies of H4SiO4, D4SiO4, H6Si2O7, and H6Si3O9 in aqueous environment, obtained from ab initio molecular dynamics. Journal of Chemical Physics, 2012, 137, 164506.	3.0	16
43	Complexation of Zr and Hf monomers in supercritical aqueous solutions: Insights from ab initio molecular dynamics simulations. Chemical Geology, 2015, 418, 30-39.	3.3	16
44	Structural and dynamical properties of supercritical H2Oâ€“SiO2 fluids studied by ab initio molecular dynamics. Chemical Geology, 2016, 426, 85-94.	3.3	16
45	Amorphous materials: Properties, structure, and durability: Atomic structure and transport properties of MgO-Al2O3 melts: A molecular dynamics simulation study. American Mineralogist, 2008, 93, 1486-1492.	1.9	15
46	Atomic scale view on partially molten rocks: Molecular dynamics simulations of melt-wetted olivine grain boundaries. Journal of Geophysical Research, 2011, 116, .	3.3	15
47	Trace element partitioning between silicate melts â€“ A molecular dynamics approach. Geochimica Et Cosmochimica Acta, 2017, 205, 245-255.	3.9	15
48	Effect of temperature on the pressure-induced spin transition in siderite and iron-bearing magnesite: a Raman spectroscopy study. European Journal of Mineralogy, 2017, 29, 785-793.	1.3	15
49	Aqueous sodium hydroxide (NaOH) solutions at high pressure and temperature: insights fromin situRaman spectroscopy andab initiomolecular dynamics simulations. Physical Chemistry Chemical Physics, 2018, 20, 21629-21639.	2.8	15
50	From Molten Calcium Aluminates through Phase Transitions to Cement Phases. Advanced Science, 2020, 7, 1902209.	11.2	15
51	Phase behavior of protoenstatite at high pressure studied by atomistic simulations. American Mineralogist, 2009, 94, 950-956.	1.9	14
52	Single-crystal elastic properties of (Y,Yb)3Al5O12. Journal of Applied Physics, 2009, 106, .	2.5	14
53	Pressure-induced hydrogen bond symmetrisation in guyanaite, Î²-CrOOH: evidence from spectroscopy and ab initio simulations. European Journal of Mineralogy, 2012, 24, 839-850.	1.3	14
54	Continuous description of a grain boundary in forsterite from atomic scale simulations: the role of disclinations. Philosophical Magazine, 2016, 96, 1757-1772.	1.6	14

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55	Copper complexation and solubility in high-temperature hydrothermal fluids: A combined study by Raman, X-ray fluorescence, and X-ray absorption spectroscopies and ab initio molecular dynamics simulations. Chemical Geology, 2018, 494, 69-79.	3.3	14
56	Atomic dynamics of alumina melt: A molecular dynamics simulation study. Condensed Matter Physics, 2008, 11, 169.	0.7	14
57	Atomic Dynamics in Liquids with Competing Interactions. Physical Review Letters, 2004, 92, 185507.	7.8	13
58	Longitudinal excitations in Mgâ€“Alâ€“O refractory oxide melts studied by inelastic x-ray scattering. Journal of Chemical Physics, 2007, 126, 114505.	3.0	12
59	Structure of liquid tricalcium aluminate. Physical Review B, 2017, 95, .	3.2	12
60	Yttrium speciation in subduction-zone fluids from ab initio molecular dynamics simulations. Solid Earth, 2020, 11, 767-789.	2.8	12
61	Cation Hydration in Supercritical NaOH and HCl Aqueous Solutions. Journal of Physical Chemistry B, 2017, 121, 11383-11389.	2.6	11
62	Strontium complexation in aqueous solutions and silicate glasses: Insights from high energy-resolution fluorescence detection X-ray spectroscopy and ab - initio modeling. Geochimica Et Cosmochimica Acta, 2014, 142, 535-552.	3.9	10
63	Fast ionic mobility in cryolite studied by quasielastic neutron scattering. Solid State Ionics, 2008, 179, 1957-1961.	2.7	9
64	Thermodynamic properties of anhydrous and hydrous wadsleyite, Î²â˜Mg₂SiO₄. High Pressure Research, 2013, 33, 584-594.	1.2	9
65	Interpretation of Raman spectra of the zirconâ€“hafnon solid solution. European Journal of Mineralogy, 2016, 28, 721-733.	1.3	9
66	From atomic structure to excess entropy: a neutron diffraction and density functional theory study of CaOâ˜Al₂O₃â˜SiO₂melts. Journal of Physics Condensed Matter, 2016, 28, 135102.	1.8	9
67	Effects of hydrostaticity on the structural stability of carbonates at lower mantle pressures: the case study of dolomite. High Pressure Research, 2019, 39, 36-49.	1.2	9
68	Anomalous elastic behavior of phase egg, AlSiO3(OH), at high pressures. American Mineralogist, 2019, 104, 130-139.	1.9	7
69	The Brillouin spectrometer BRISP at the ILL. Physica B: Condensed Matter, 2006, 385-386, 1092-1094.	2.7	6
70	Sodium diffusion in cryolite at elevated temperatures studied by quasielastic neutron scattering. Solid State Ionics, 2009, 180, 1257-1260.	2.7	6
71	Integral modeling approach to study the phase behavior of complex solids: application to phase transitions in MgSiO₃pyroxenes. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, 535-541.	0.3	6
72	Insights from X-ray absorption/fluorescence spectroscopy and ab-initio molecular dynamics on concentration and complexa-tion of Zr and Hf in aqueous fluids at high pressure and temperature. Journal of Physics: Conference Series, 2013, 430, 012122.	0.4	6

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73	Anisotropy of self-diffusion in forsterite grain boundaries derived from molecular dynamics simulations. Contributions To Mineralogy and Petrology, 2016, 171, 1.	3.1	6
74	Exchange-correlation functional dependence of the O 1s excitation spectrum of water. Journal of Electron Spectroscopy and Related Phenomena, 2018, 222, 57-62.	1.7	6
75	Monte-Carlo simulation of a neutron Brillouin scattering spectrometer. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 1999, 438, 452-459.	1.6	5
76	The atomic dynamics of liquid Rb x Sb 1-x. Applied Physics A: Materials Science and Processing, 2002, 74, s1664-s1666.	2.3	5
77	Atomic dynamics in liquid KxSb1â^'x alloys. Journal of Non-Crystalline Solids, 2007, 353, 3145-3148.	3.1	5
78	The structure of Y- and La-bearing aluminosilicate glasses and melts: A combined molecular dynamics and diffraction study. Chemical Geology, 2017, 461, 23-33.	3.3	5
79	Ni partitioning between metal and silicate melts: An exploratory abÂinitio molecular dynamics simulation study. Chemical Geology, 2017, 461, 47-53.	3.3	5
80	Ion association in hydrothermal aqueous NaCl solutions: implications for the microscopic structure of supercritical water. Physical Chemistry Chemical Physics, 2021, 23, 14845-14856.	2.8	5
81	Experimental evidence for the bimodal character of the vibrational spectrum of Zintl -type liquids. Europhysics Letters, 2004, 67, 793-799.	2.0	4
82	The structure of liquid calcium aluminates as investigated by neutron and high-energy x-ray diffraction in combination with molecular dynamics simulation methods. Journal of Physics Condensed Matter, 2012, 24, 099501.	1.8	4
83	Configurational constraints on glass formation in the liquid calcium aluminate system. Journal of Statistical Mechanics: Theory and Experiment, 2019, 2019, 104012.	2.3	4
84	Effect of cationic substitution on the pressure-induced phase transitions in calcium carbonate. American Mineralogist, 2021, 106, 549-558.	1.9	4
85	Properties of irradiated sodium borosilicate glasses from experiment and atomistic simulations. Journal of the American Ceramic Society, 2021, 104, 4479-4491.	3.8	4
86	Molecular Simulations of Oxide and Silicate Melts and Glasses. Reviews in Mineralogy and Geochemistry, 2022, 87, 193-227.	4.8	4
87	The microscopic dynamics of liquid NaxSn1â^'x. Journal of Non-Crystalline Solids, 2002, 312-314, 134-137.	3.1	3
88	Monte-Carlo simulation of a single monochromator neutron Brillouin spectrometer. Applied Physics A: Materials Science and Processing, 2002, 74, s1465-s1467.	2.3	3
89	Progress on the construction of the thermal neutron scattering spectrometer BRISP. Physica B: Condensed Matter, 2004, 350, E795-E797.	2.7	3
90	Structure of levitated Siâ€“Ge melts studied by high-energy x-ray diffraction in combination with reverse Monte Carlo simulations. Journal of Physics Condensed Matter, 2021, 33, 244002.	1.8	3

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91	Collective atomic dynamics in molten Rb(100â^'x)Sbx investigated by inelastic neutron scattering. Journal of Non-Crystalline Solids, 1999, 250-252, 263-266.	3.1	2
92	17. Theoretical Approaches to Structure and Spectroscopy of Earth Materials. , 2014, , 691-744.		1
93	"Non-simple liquids" - a challenge for neutron Brillouin scattering?. Journal of Neutron Research, 2006, 14, 297-302.	1.1	0
94	Single and collective particle dynamics in liquid Rb80(RbBr)20. Journal of Physics: Conference Series, 2008, 98, 022002.	0.4	0
95	Atomic-scale modelling of crystal defects, self-diffusion and deformation processes. , 2017, , 215-253.		0
96	Hydration in aqueous NaCl. Physical Chemistry Chemical Physics, 0, , .	2.8	0