Razvan Caracas

List of Publications by Year in Descending Order

97 papers	6,856 citations	30 h-index	82 g-index
108 ext. papers	7,479 ext. citations	4.5 avg, IF	5.49 L-index

#	Paper	IF	Citations
97	Genesis of a CO-rich and HO-depleted atmosphere from Earth's early global magma ocean. *Science Advances*, **2021**, 7, eabj0406	14.3	0
96	Gibbs ensemble Monte Carlo simulations of the liquid-vapor equilibrium and the critical point of sodium. *Physical Chemistry Chemical Physics*, **2021**, 23, 311-319	3.6	
95	Buoyancy and Structure of Volatile-Rich Silicate Melts. *Journal of Geophysical Research: Solid Earth*, **2021**, 126, e2020JB021045	3.6	5
94	Analyzing Melts and Fluids from Ab Initio Molecular Dynamics Simulations with the UMD Package. *Journal of Visualized Experiments*, **2021**,	1.6	1
93	Thermophysical properties of hot fluid iron in the protolunar disk. *Physics of the Earth and Planetary Interiors*, **2021**, 321, 106806	2.3	
92	The Critical Point and the Supercritical State of Alkali Feldspars: Implications for the Behavior of the Crust During Impacts. *Journal of Geophysical Research E: Planets*, **2020**, 125, e2020JE006412	4.1	4
91	Carbon Speciation and Solubility in Silicate Melts. *Geophysical Monograph Series*, **2020**, 179-194	1.1	5
90	Partial core vaporization during Giant Impacts inferred from the entropy and the critical point of iron. *Earth and Planetary Science Letters*, **2020**, 547, 116463	5.3	2
89	Stability and Solid Solutions of Hydrous Alumino-Silicates in the Earth□ Mantle. *Minerals (Basel, Switzerland)*, **2020**, 10, 330	2.4	1
88	Melt□rystal density crossover in a deep magma ocean. *Earth and Planetary Science Letters*, **2019**, 516, 202-211	5.3	30
87	Projector augmented-wave formulation of response to strain and electric-field perturbation within density functional perturbation theory. *Physical Review B*, **2019**, 99,	3.3	3
86	Pressure-Induced Coordination Changes in a Pyrolitic Silicate Melt From Ab Initio Molecular Dynamics Simulations. *Journal of Geophysical Research: Solid Earth*, **2019**, 124, 11232-11250	3.6	11
85	Carbon sequestration during core formation implied by complex carbon polymerization. *Nature Communications*, **2019**, 10, 789	17.4	17
84	High-pressure yield strength of rocksalt structures using quartz Raman piezometry. *Comptes Rendus - Geoscience*, **2019**, 351, 71-79	1.4	3
83	Anharmonic contribution to the stabilization of Mg(OH) from first principles. *Physical Chemistry Chemical Physics*, **2018**, 20, 17799-17808	3.6	6
82	Proton dynamics and the phase diagram of dense water ice. *Journal of Chemical Physics*, **2018**, 148, 214501	3.9	33
81	Stability of phase H in the MgSiO 4 H 2 □lOOH□iO 2 system. *Earth and Planetary Science Letters*, **2017**, 463, 171-177	5.3	24

80	Salt partitioning between water and high-pressure ices. Implication for the dynamics and habitability of icy moons and water-rich planetary bodies. *Earth and Planetary Science Letters*, **2017**, 463, 36-47	5.3	24
79	Compressional pathways of □cristobalite, structure of cristobalite X-I, and towards the understanding of seifertite formation. *Nature Communications*, **2017**, 8, 15647	17.4	19
78	The influence of carbon on the seismic properties of solid iron. *Geophysical Research Letters*, **2017**, 44, 128-134	4.9	11
77	Reconciling magma-ocean crystallization models with the present-day structure of the Earth's mantle. *Geochemistry, Geophysics, Geosystems*, **2017**, 18, 2785-2806	3.6	41
76	Hydrogen mobility in transition zone silicates. *Progress in Earth and Planetary Science*, **2017**, 4,	3.9	6
75	High-pressure behavior of □boron studied on single crystals by X-ray diffraction, Raman and IR spectroscopy. *Journal of Solid State Chemistry*, **2017**, 245, 50-60	3.3	7
74	Sound velocities of bridgmanite from density of states determined by nuclear inelastic scattering and first-principles calculations. *Progress in Earth and Planetary Science*, **2016**, 3,	3.9	5
73	High-pressure compressibility and vibrational properties of (Ca,Mn)CO3. *American Mineralogist*, **2016**, 101, 2723-2730	2.9	17
72	Pressure-dependent isotopic composition of iron alloys. *Science*, **2016**, 352, 580-2	33.3	53
71	Superionic-Superionic Phase Transitions in Body-Centered Cubic H_{2}O Ice. *Physical Review Letters*, **2016**, 117, 135503	7.4	36
70	Crystal Structures of Core Materials. *Geophysical Monograph Series*, **2016**, 55-68	1.1	4
69	Lattice Vibrations and Spectroscopy of Mantle Phases **2015**, 203-231		1
68	Serpentines, talc, chlorites, and their high-pressure phase transitions: a Raman spectroscopic study. *Physics and Chemistry of Minerals*, **2015**, 42, 641-649	1.6	16
67	Ferroelectricity in high-density H2O ice. *Journal of Chemical Physics*, **2015**, 142, 134501	3.9	6
66	The influence of hydrogen on the seismic properties of solid iron. *Geophysical Research Letters*, **2015**, 42, 3780-3785	4.9	28
65	Elasticity and dislocations in ice X under pressure. *Physics of the Earth and Planetary Interiors*, **2014**, 236, 10-15	2.3	17
64	Identifying the spin transition in Fe2+-rich MgSiO3 perovskite from X-ray diffraction and vibrational spectroscopy. *American Mineralogist*, **2014**, 99, 1270-1276	2.9	6
63	Stability and spectroscopy of Mg sulfate minerals: Role of hydration on sulfur isotope partitioning. *American Mineralogist*, **2014**, 99, 1216-1220	2.9	0

62	Equations of state in the Fe-FeSi system at high pressures and temperatures. *Journal of Geophysical Research: Solid Earth*, **2014**, 119, 2810-2827	3.6	52
61	Chemistry and Mineralogy of Earth's Mantle. Hexagonal Na0.41[Na0.125Mg0.79Al0.085]2[Al0.79Si0.21]6O12 (NAL phase): Crystal structure refinement and elasticity. *American Mineralogist*, **2014**, 99, 1562-1569	2.9	10
60	Pressure-induced phase transitions in coesite. *American Mineralogist*, **2014**, 99, 755-763	2.9	13
59	The high conductivity of iron and thermal evolution of the Earth's core. *Physics of the Earth and Planetary Interiors*, **2013**, 224, 88-103	2.3	209
58	Raman spectroscopic properties and Raman identification of CaS-MgS-MnS-FeS-Cr2FeS4 sulfides in meteorites and reduced sulfur-rich systems. *Meteoritics and Planetary Science*, **2013**, 48, 1415-1426	2.8	48
57	Influence of NaCl on ice VI and ice VII melting curves up to 6 GPa, implications for large icy moons. *Icarus*, **2013**, 226, 355-363	3.8	31
56	Anharmonicity of graphite from UV Raman spectroscopy to 2700 K. *Carbon*, **2013**, 54, 68-75	10.4	18
55	Elasticity and lattice dynamics of enstatite at high pressure. *Journal of Geophysical Research: Solid Earth*, **2013**, 118, 4071-4082	3.6	22
54	Raman spectroscopy investigation of alpha boron at elevated pressures and temperatures. *Solid State Communications*, **2013**, 154, 34-39	1.6	20
53	First-Principles Calculations of Physical Properties of Planetary Ices. *Astrophysics and Space Science Library*, **2013**, 149-169	0.3	
52	Effect of chemistry on the compressibility of silicate perovskite in the lower mantle. *Earth and Planetary Science Letters*, **2012**, 333-334, 181-190	5.3	64
51	Creep of phyllosilicates at the onset of plate tectonics. *Earth and Planetary Science Letters*, **2012**, 345-348, 142-150	5.3	52
50	Equation of state and phase diagram of Fe16Si alloy as a candidate component of Earth's core. *Earth and Planetary Science Letters*, **2012**, 357-358, 268-276	5.3	45
49	Bonding and structural changes in siderite at high pressure. *American Mineralogist*, **2012**, 97, 1421-1426	2.9	30
48	The WURM project: a freely available web-based repository of computed physical data for minerals. *American Mineralogist*, **2011**, 96, 437-443	2.9	34
47	Is the spin transition in Fe2+-bearing perovskite visible in seismology?. *Geophysical Research Letters*, **2010**, 37, n/a-n/a	4.9	12
46	Elasticity of AlFeO3 and FeAlO3 perovskite and post-perovskite from first-principles calculations. *Geophysical Research Letters*, **2010**, 37, n/a-n/a	4.9	8
45	Elasticity of (K,Na)AlSi3O8 hollandite from lattice dynamics calculations. *Physics of the Earth and Planetary Interiors*, **2010**, 181, 21-26	2.3	24

44	Spin and structural transitions in AlFeO3 and FeAlO3 perovskite and post-perovskite. *Physics of the Earth and Planetary Interiors*, **2010**, 182, 10-17	2.3	22
43	Theoretical determination of the Raman spectra of single-crystal forsterite (Mg2SiO4). *American Mineralogist*, **2010**, 95, 980-986	2.9	25
42	Diamond as a high pressure gauge up to 2.7 Mbar. *Applied Physics Letters*, **2010**, 97, 251903	3.4	25
41	Ab Initio Lattice Dynamics and Thermodynamical Properties **2010**, 291-315		1
40	Pressure-induced isostructural phase transformation in □B28. *Physical Review B*, **2010**, 82,	3.3	26
39	High-pressure ferroelastic phase transition in aluminosilicate hollandite. *Physical Review B*, **2009**, 80,	3.3	11
38	ABINIT: First-principles approach to material and nanosystem properties. *Computer Physics Communications*, **2009**, 180, 2582-2615	4.2	2006
37	D/H isotopic fractionation between brucite Mg(OH)2 and water from first-principles vibrational modeling. *Chemical Geology*, **2009**, 262, 159-168	4.2	27
36	Advances in experimental and theoretical isotope geochemistry. *Chemical Geology*, **2009**, 267, 109-110	4.2	2
35	Elasticity and Raman and infrared spectra of MgAl2O4 spinel from density functional perturbation theory. *Physics of the Earth and Planetary Interiors*, **2009**, 174, 113-121	2.3	38
34	Ferrous iron in post-perovskite from first-principles calculations. *Physics of the Earth and Planetary Interiors*, **2008**, 168, 147-152	2.3	37
33	Synchrotron infrared spectroscopy of the pressure-induced insulator-metal transitions in glassy As2S3 and As2Se3. *Physical Review B*, **2008**, 77,	3.3	24
32	Dynamical instabilities of ice X. *Physical Review Letters*, **2008**, 101, 085502	7.4	61
31	X-Ray Induced Synthesis of 8H Diamond. *Advanced Materials*, **2008**, 20, 3303-3307	24	22
30	New structures of dense nitrogen: Pathways to the polymeric phase. *Chemical Physics Letters*, **2007**, 442, 65-70	2.5	26
29	Raman spectra and lattice dynamics of cubic gauche nitrogen. *Journal of Chemical Physics*, **2007**, 127, 144510	3.9	31
28	Post-perovskite phase in selected sesquioxides from density-functional calculations. *Physical Review B*, **2007**, 76,	3.3	23
27	Prediction of polar ordered oxynitride perovskites. *Applied Physics Letters*, **2007**, 91, 092902	3.4	15

26	Effect of chemistry on the physical properties of perovskite and post-perovskite. *Geophysical Monograph Series*, **2007**, 115-128	1.1	12
25	Theoretical determination of the Raman spectra of MgSiO3 perovskite and post-perovskite at high pressure. *Geophysical Research Letters*, **2006**, 33,	4.9	29
24	First-principles study of high-temperature phases of K2SeO4. *Physical Review B*, **2006**, 74,	3.3	2
23	Elasticity of CaSiO3 perovskite at high pressure and high temperature. *Physics of the Earth and Planetary Interiors*, **2006**, 155, 249-259	2.3	72
22	Phase stability of CaSiO3 perovskite at high pressure and temperature: Insights from ab initio molecular dynamics. *Physics of the Earth and Planetary Interiors*, **2006**, 155, 260-268	2.3	40
21	Theoretical determination of the structures of CaSiO3 perovskites. *Acta Crystallographica Section B: Structural Science*, **2006**, 62, 1025-30		15
20	First-principle studies of the lattice dynamics of crystals, and related properties. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2005**, 220,	1	55
19	First-principles determination of the dynamical properties of Pb2MgTeO6. *Physical Review B*, **2005**, 71,	3.3	3
18	CaSiO3 perovskite at lower mantle pressures. *Geophysical Research Letters*, **2005**, 32,	4.9	42
17	Prediction of a new phase transition in Al2O3 at high pressures. *Geophysical Research Letters*, **2005**, 32,	4.9	44
16	Effect of chemistry on the stability and elasticity of the perovskite and post-perovskite phases in the MgSiO3-FeSiO3-Al2O3 system and implications for the lowermost mantle. *Geophysical Research Letters*, **2005**, 32,	4.9	94
15	First-principle study of materials involved in incommensurate transitions. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2005**, 220,	1	8
14	First-principles study of the electronic properties of A2B3 minerals, with A=Bi,Sb and B=S,Se. *Physics and Chemistry of Minerals*, **2005**, 32, 295-300	1.6	88
13	Iron-rich silicates in the Earth's D'' layer. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 9751-3	11.5	92
12	High-pressure isosymmetrical phase transition in calaverite. *Physics and Chemistry of Minerals*, **2004**, 31, 553-558	1.6	
11	First principles determination of the phase boundaries of high-pressure polymorphs of silica. *Geophysical Research Letters*, **2004**, 31, n/a-n/a	4.9	63
10	Equation of state and elasticity of FeSi. *Geophysical Research Letters*, **2004**, 31,	4.9	40
9	Structural, electronic, and dynamical properties of calaverite AuTe2 under pressure. *Physical Review B*, **2004**, 69,	3.3	5

8	First-principles calculations of K2SeO4 dielectrics. *AIP Conference Proceedings*, **2003**,	0	1
7	Ab initio determination of the ground-state properties of Ca2MgSi2O7 åkermanite. *Physical Review B*, **2003**, 68,	3.3	18
6	A database of incommensurate phases. *Journal of Applied Crystallography*, **2002**, 35, 120-121	3.8	8
5	First-principles study of Pb2MgTeO6: High-T cubic phase and average low-T rhombohedral phase. *Physical Review B*, **2002**, 65,	3.3	4
4	First-principles computation of material properties: the ABINIT software project. *Computational Materials Science*, **2002**, 25, 478-492	3.2	2556
3	Ab initio determination of the valence electron distribution in the average structure of the incommensurately modulated calaverite AuTe2. *Acta Crystallographica Section B: Structural Science*, **2001**, 57, 633-7		4
2	Ab initio study of incommensurately modulated crystals. *Computational Materials Science*, **2001**, 22, 112-117	1.1	1
1	Theoretical modelling of Raman spectra173-191		1