

Razvan Caracas

List of Publications by Year in descending order

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99
papers

8,046
citations

109137

35
h-index

46693

89
g-index

108
all docs

108
docs citations

108
times ranked

7484
citing authors

#	ARTICLE	IF	CITATIONS
1	First-principles computation of material properties: the ABINIT software project. Computational Materials Science, 2002, 25, 478-492.	1.4	2,789
2	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	3.0	2,297
3	The high conductivity of iron and thermal evolution of the Earth's core. Physics of the Earth and Planetary Interiors, 2013, 224, 88-103.	0.7	251
4	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.	0.3	109
5	Iron-rich silicates in the Earth's D'' layer. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 9751-9753.	3.3	100
6	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, .	1.5	100
7	Elasticity of CaSiO3 perovskite at high pressure and high temperature. Physics of the Earth and Planetary Interiors, 2006, 155, 249-259.	0.7	84
8	First principles determination of the phase boundaries of high-pressure polymorphs of silica. Geophysical Research Letters, 2004, 31, n/a-n/a.	1.5	80
9	Effect of chemistry on the compressibility of silicate perovskite in the lower mantle. Earth and Planetary Science Letters, 2012, 333-334, 181-190.	1.8	78
10	First-principle studies of the lattice dynamics of crystals, and related properties. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.4	72
11	Dynamical Instabilities of Ice X. Physical Review Letters, 2008, 101, 085502.	2.9	72
12	Equations of state in the Fe-FeSi system at high pressures and temperatures. Journal of Geophysical Research: Solid Earth, 2014, 119, 2810-2827.	1.4	71
13	Raman spectroscopic properties and Raman identification of Ca-Mg-Mn-Fe-Cr ₂ FeS ₄ sulfides in meteorites and reduced sulfur-rich systems. Meteoritics and Planetary Science, 2013, 48, 1415-1426.	0.7	68
14	Pressure-dependent isotopic composition of iron alloys. Science, 2016, 352, 580-582.	6.0	68
15	Creep of phyllosilicates at the onset of plate tectonics. Earth and Planetary Science Letters, 2012, 345-348, 142-150.	1.8	59
16	Reconciling magma-ocean crystallization models with the present-day structure of the Earth's mantle. Geochemistry, Geophysics, Geosystems, 2017, 18, 2785-2806.	1.0	58
17	CaSiO3 perovskite at lower mantle pressures. Geophysical Research Letters, 2005, 32, .	1.5	57
18	Equation of state and phase diagram of Fe-16Si alloy as a candidate component of Earth's core. Earth and Planetary Science Letters, 2012, 357-358, 268-276.	1.8	55

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19	Meltâ€“crystal density crossover in a deep magma ocean. Earth and Planetary Science Letters, 2019, 516, 202-211.	1.8	54
20	Superionic-Superionic Phase Transitions in Body-Centered Cubic H_2O . Physical Review Letters, 2016, 117, 135503.	2.9	53
21	Equation of state and elasticity of FeSi. Geophysical Research Letters, 2004, 31, .	1.5	52
22	Prediction of a new phase transition in Al_2O_3 at high pressures. Geophysical Research Letters, 2005, 32, .	1.5	50
23	The WURM project—a freely available web-based repository of computed physical data for minerals. American Mineralogist, 2011, 96, 437-443.	0.9	48
24	Proton dynamics and the phase diagram of dense water ice. Journal of Chemical Physics, 2018, 148, 214501.	1.2	48
25	Phase stability of CaSiO_3 perovskite at high pressure and temperature: Insights from ab initio molecular dynamics. Physics of the Earth and Planetary Interiors, 2006, 155, 260-268.	0.7	46
26	Elasticity and Raman and infrared spectra of MgAl_2O_4 spinel from density functional perturbation theory. Physics of the Earth and Planetary Interiors, 2009, 174, 113-121.	0.7	46
27	Bonding and structural changes in siderite at high pressure. American Mineralogist, 2012, 97, 1421-1426.	0.9	45
28	Influence of NaCl on ice VI and ice VII melting curves up to 6GPa, implications for large icy moons. Icarus, 2013, 226, 355-363.	1.1	42
29	Raman spectra and lattice dynamics of cubic <i>gauche</i> nitrogen. Journal of Chemical Physics, 2007, 127, 144510.	1.2	40
30	Ferrous iron in post-perovskite from first-principles calculations. Physics of the Earth and Planetary Interiors, 2008, 168, 147-152.	0.7	40
31	The influence of hydrogen on the seismic properties of solid iron. Geophysical Research Letters, 2015, 42, 3780-3785.	1.5	40
32	Theoretical determination of the Raman spectra of MgSiO_3 perovskite and post-perovskite at high pressure. Geophysical Research Letters, 2006, 33, .	1.5	39
33	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.	1.8	39
34	Theoretical determination of the Raman spectra of single-crystal forsterite (Mg_2SiO_4). American Mineralogist, 2010, 95, 980-986.	0.9	38
35	D/H isotopic fractionation between brucite $\text{Mg}(\text{OH})_2$ and water from first-principles vibrational modeling. Chemical Geology, 2009, 262, 159-168.	1.4	37
36	Compressional pathways of $\hat{\Gamma}$ -cristobalite, structure of cristobalite X-I, and towards the understanding of seifertite formation. Nature Communications, 2017, 8, 15647.	5.8	33

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37	New structures of dense nitrogen: Pathways to the polymeric phase. <i>Chemical Physics Letters</i> , 2007, 442, 65-70.	1.2	31
38	Stability of phase H in the MgSiO ₄ -H ₂ O-AlOOH-SiO ₂ system. <i>Earth and Planetary Science Letters</i> , 2017, 463, 171-177.	1.8	31
39	Diamond as a high pressure gauge up to 2.7 Mbar. <i>Applied Physics Letters</i> , 2010, 97, .	1.5	29
40	Elasticity and lattice dynamics of enstatite at high pressure. <i>Journal of Geophysical Research: Solid Earth</i> , 2013, 118, 4071-4082.	1.4	29
41	High-pressure compressibility and vibrational properties of (Ca,Mn)CO ₃ . <i>American Mineralogist</i> , 2016, 101, 2723-2730.	0.9	29
42	Post-perovskite phase in selected sesquioxides from density-functional calculations. <i>Physical Review B</i> , 2007, 76, .	1.1	27
43	Pressure-induced isostructural phase transformation in $\text{In}^3\text{-B28}$. <i>Physical Review B</i> , 2010, 82, .	1.1	27
44	Raman spectroscopy investigation of alpha boron at elevated pressures and temperatures. <i>Solid State Communications</i> , 2013, 154, 34-39.	0.9	27
45	Pressure-Induced Coordination Changes in a Pyrolytic Silicate Melt From Ab Initio Molecular Dynamics Simulations. <i>Journal of Geophysical Research: Solid Earth</i> , 2019, 124, 11232-11250.	1.4	27
46	Carbon sequestration during core formation implied by complex carbon polymerization. <i>Nature Communications</i> , 2019, 10, 789.	5.8	27
47	Synchrotron infrared spectroscopy of the pressure-induced insulator-metal transitions in glassy As_2S_3 and As_2Se_3 . <i>Physical Review B</i> , 2019, 100, 040401.	1.1	26
48	Elasticity of (K,Na)AlSi ₃ O ₈ hollandite from lattice dynamics calculations. <i>Physics of the Earth and Planetary Interiors</i> , 2010, 181, 21-26.	0.7	24
49	Spin and structural transitions in AlFeO ₃ and FeAlO ₃ perovskite and post-perovskite. <i>Physics of the Earth and Planetary Interiors</i> , 2010, 182, 10-17.	0.7	24
50	X-Ray Induced Synthesis of 8H Diamond. <i>Advanced Materials</i> , 2008, 20, 3303-3307.	11.1	22
51	Serpentines, talc, chlorites, and their high-pressure phase transitions: a Raman spectroscopic study. <i>Physics and Chemistry of Minerals</i> , 2015, 42, 641-649.	0.3	21
52	Theoretical determination of the structures of CaSiO ₃ perovskites. <i>Acta Crystallographica Section B: Structural Science</i> , 2006, 62, 1025-1030.	1.8	20
53	Ab initio determination of the ground-state properties of Ca ₂ MgSi ₂ O ₇ kermanite. <i>Physical Review B</i> , 2003, 68, .	1.1	18
54	Prediction of polar ordered oxynitride perovskites. <i>Applied Physics Letters</i> , 2007, 91, .	1.5	18

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55	Is the spin transition in Fe ²⁺ -bearing perovskite visible in seismology?. Geophysical Research Letters, 2010, 37, .	1.5	18
56	Anharmonicity of graphite from UV Raman spectroscopy to 2700K. Carbon, 2013, 54, 68-75.	5.4	18
57	Elasticity and dislocations in ice X under pressure. Physics of the Earth and Planetary Interiors, 2014, 236, 10-15.	0.7	18
58	Pressure-induced phase transitions in coesite. American Mineralogist, 2014, 99, 755-763.	0.9	16
59	The influence of carbon on the seismic properties of solid iron. Geophysical Research Letters, 2017, 44, 128-134.	1.5	15
60	Buoyancy and Structure of Volatile-Rich Silicate Melts. Journal of Geophysical Research: Solid Earth, 2021, 126, e2020JB021045.	1.4	14
61	High-pressure ferroelastic phase transition in aluminosilicate hollandite. Physical Review B, 2009, 80, .	1.1	13
62	Hydrogen mobility in transition zone silicates. Progress in Earth and Planetary Science, 2017, 4, .	1.1	13
63	Stability of high-temperature salty ice suggests electrolyte permeability in water-rich exoplanet icy mantles. Nature Communications, 2022, 13, .	5.8	13
64	Effect of chemistry on the physical properties of perovskite and post-perovskite. Geophysical Monograph Series, 2007, , 115-128.	0.1	12
65	Hexagonal Na _{0.41} [Na _{0.125} Mg _{0.79} Al _{0.085}] ₂ [Al _{0.79} Si _{0.21}] ₆ O ₁₂ (NAL phase): Crystal structure refinement and elasticity. American Mineralogist, 2014, 99, 1562-1569.	0.9	10
66	Identifying the spin transition in Fe ²⁺ -rich MgSiO ₃ perovskite from X-ray diffraction and vibrational spectroscopy. American Mineralogist, 2014, 99, 1270-1276.	0.9	10
67	Anharmonic contribution to the stabilization of Mg(OH) ₂ from first principles. Physical Chemistry Chemical Physics, 2018, 20, 17799-17808.	1.3	10
68	Elasticity of AlFeO ₃ and FeAlO ₃ perovskite and post-perovskite from first-principles calculations. Geophysical Research Letters, 2010, 37, .	1.5	9
69	High-pressure behavior of ¹¹ B studied on single crystals by X-ray diffraction, Raman and IR spectroscopy. Journal of Solid State Chemistry, 2017, 245, 50-60.	1.4	9
70	Projector augmented-wave formulation of response to strain and electric-field perturbation within density functional perturbation theory. Physical Review B, 2019, 99, .	1.1	9
71	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.	1.5	9
72	Genesis of a CO ₂ -rich and H ₂ O-depleted atmosphere from Earth's early global magma ocean. Science Advances, 2021, 7, eabj0406.	4.7	9

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73	A database of incommensurate phases. <i>Journal of Applied Crystallography</i> , 2002, 35, 120-121.	1.9	8
74	First-principle study of materials involved in incommensurate transitions. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2005, 220, .	0.4	8
75	Structural, electronic, and dynamical properties of calaverite AuTe_2 under pressure. <i>Physical Review B</i> , 2004, 69, .	1.1	7
76	Partial core vaporization during Giant Impacts inferred from the entropy and the critical point of iron. <i>Earth and Planetary Science Letters</i> , 2020, 547, 116463.	1.8	7
77	Ab initio determination of the valence electron distribution in the average structure of the incommensurately modulated calaverite AuTe_2 . <i>Acta Crystallographica Section B: Structural Science</i> , 2001, 57, 633-637.	1.8	6
78	Ferroelectricity in high-density H_2O ice. <i>Journal of Chemical Physics</i> , 2015, 142, 134501.	1.2	6
79	Sound velocities of bridgmanite from density of states determined by nuclear inelastic scattering and first-principles calculations. <i>Progress in Earth and Planetary Science</i> , 2016, 3, .	1.1	6
80	Critical point and supercritical regime of MgO . <i>Physical Review B</i> , 2022, 105, .	1.1	6
81	First-principles study of $\text{Pb}_2\text{MgTeO}_6$: High-T cubic phase and average low-T rhombohedral phase. <i>Physical Review B</i> , 2002, 65, .	1.1	4
82	High-pressure yield strength of rocksalt structures using quartz Raman piezometry. <i>Comptes Rendus - Geoscience</i> , 2019, 351, 71-79.	0.4	4
83	Stability and Solid Solutions of Hydrous Alumino-Silicates in the Earth's Mantle. <i>Minerals (Basel)</i> , 2021, 11, 1078.	0.8	4
84	The Speciation and Coordination of a Deep Earth Carbonate-Silicate-Metal Melt. <i>Journal of Geophysical Research: Solid Earth</i> , 2022, 127, .	1.4	4
85	First-principles determination of the dynamical properties of $\text{Pb}_2\text{MgTeO}_6$. <i>Physical Review B</i> , 2005, 71, .	1.1	3
86	Lattice Vibrations and Spectroscopy of Mantle Phases. , 2015, , 203-231.		3
87	Analyzing Melts and Fluids from Ab Initio Molecular Dynamics Simulations with the UMD Package. <i>Journal of Visualized Experiments</i> , 2021, , .	0.2	3
88	First-principles study of high-temperature phases of K_2SeO_4 . <i>Physical Review B</i> , 2006, 74, .	1.1	2
89	Advances in experimental and theoretical isotope geochemistry. <i>Chemical Geology</i> , 2009, 267, 109-110.	1.4	2
90	Stability and spectroscopy of Mg sulfate minerals: Role of hydration on sulfur isotope partitioning. <i>American Mineralogist</i> , 2014, 99, 1216-1220.	0.9	2

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91	Ab initio study of the structure and relative stability of MgSiO ₄ H ₂ polymorphs at high pressures and temperatures. American Mineralogist, 2022, 107, 781-789.	0.9	2
92	Ab initio study of incommensurately modulated crystals. Computational Materials Science, 2001, 22, 112-117.	1.4	1
93	Ab initio Lattice Dynamics of Pb ₂ MgTeO ₆ Double Perovskite. AIP Conference Proceedings, 2002, , .	0.3	1
94	First-principles calculations of K ₂ SeO ₄ dielectrics. AIP Conference Proceedings, 2003, , .	0.3	1
95	Theoretical modelling of Raman spectra. , 0, , 173-191.		1
96	High-pressure isosymmetrical phase transition in calaverite. Physics and Chemistry of Minerals, 2004, 31, 553-558.	0.3	0
97	<i>Ab initio</i> Gibbs ensemble Monte Carlo simulations of the liquid-vapor equilibrium and the critical point of sodium. Physical Chemistry Chemical Physics, 2021, 23, 311-319.	1.3	0
98	Thermophysical properties of hot fluid iron in the protolunar disk. Physics of the Earth and Planetary Interiors, 2021, 321, 106806.	0.7	0
99	First-Principles Calculations of Physical Properties of Planetary Ices. Astrophysics and Space Science Library, 2013, , 149-169.	1.0	0