

Razvan Caracas

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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	First-principles computation of material properties: the ABINIT software project. <i>Computational Materials Science</i> , 2002 , 25, 478-492	3.2	2556
96	ABINIT: First-principles approach to material and nanosystem properties. <i>Computer Physics Communications</i> , 2009 , 180, 2582-2615	4.2	2006
95	The high conductivity of iron and thermal evolution of the Earth's core. <i>Physics of the Earth and Planetary Interiors</i> , 2013 , 224, 88-103	2.3	209
94	Effect of chemistry on the stability and elasticity of the perovskite and post-perovskite phases in the MgSiO ₃ -FeSiO ₃ -Al ₂ O ₃ system and implications for the lowermost mantle. <i>Geophysical Research Letters</i> , 2005 , 32,	4.9	94
93	Iron-rich silicates in the Earth's D'' layer. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005 , 102, 9751-3	11.5	92
92	First-principles study of the electronic properties of A ₂ B ₃ minerals, with A=Bi,Sb and B=S,Se. <i>Physics and Chemistry of Minerals</i> , 2005 , 32, 295-300	1.6	88
91	Elasticity of CaSiO ₃ perovskite at high pressure and high temperature. <i>Physics of the Earth and Planetary Interiors</i> , 2006 , 155, 249-259	2.3	72
90	Effect of chemistry on the compressibility of silicate perovskite in the lower mantle. <i>Earth and Planetary Science Letters</i> , 2012 , 333-334, 181-190	5.3	64
89	First principles determination of the phase boundaries of high-pressure polymorphs of silica. <i>Geophysical Research Letters</i> , 2004 , 31, n/a-n/a	4.9	63
88	Dynamical instabilities of ice X. <i>Physical Review Letters</i> , 2008 , 101, 085502	7.4	61
87	First-principle studies of the lattice dynamics of crystals, and related properties. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2005 , 220,	1	55
86	Pressure-dependent isotopic composition of iron alloys. <i>Science</i> , 2016 , 352, 580-2	33.3	53
85	Equations of state in the Fe-FeSi system at high pressures and temperatures. <i>Journal of Geophysical Research: Solid Earth</i> , 2014 , 119, 2810-2827	3.6	52
84	Creep of phyllosilicates at the onset of plate tectonics. <i>Earth and Planetary Science Letters</i> , 2012 , 345-348, 142-150	5.3	52
83	Raman spectroscopic properties and Raman identification of CaS-MgS-MnS-FeS-Cr ₂ FeS ₄ sulfides in meteorites and reduced sulfur-rich systems. <i>Meteoritics and Planetary Science</i> , 2013 , 48, 1415-1426	2.8	48
82	Equation of state and phase diagram of Fe ₁₆ Si alloy as a candidate component of Earth's core. <i>Earth and Planetary Science Letters</i> , 2012 , 357-358, 268-276	5.3	45
81	Prediction of a new phase transition in Al ₂ O ₃ at high pressures. <i>Geophysical Research Letters</i> , 2005 , 32,	4.9	44

80	CaSiO ₃ perovskite at lower mantle pressures. <i>Geophysical Research Letters</i> , 2005 , 32,	4.9	42
79	Reconciling magma-ocean crystallization models with the present-day structure of the Earth's mantle. <i>Geochemistry, Geophysics, Geosystems</i> , 2017 , 18, 2785-2806	3.6	41
78	Phase stability of CaSiO ₃ perovskite at high pressure and temperature: Insights from ab initio molecular dynamics. <i>Physics of the Earth and Planetary Interiors</i> , 2006 , 155, 260-268	2.3	40
77	Equation of state and elasticity of FeSi. <i>Geophysical Research Letters</i> , 2004 , 31,	4.9	40
76	Elasticity and Raman and infrared spectra of MgAl ₂ O ₄ spinel from density functional perturbation theory. <i>Physics of the Earth and Planetary Interiors</i> , 2009 , 174, 113-121	2.3	38
75	Ferrous iron in post-perovskite from first-principles calculations. <i>Physics of the Earth and Planetary Interiors</i> , 2008 , 168, 147-152	2.3	37
74	Superionic-Superionic Phase Transitions in Body-Centered Cubic H ₂ O Ice. <i>Physical Review Letters</i> , 2016 , 117, 135503	7.4	36
73	The WURM project: freely available web-based repository of computed physical data for minerals. <i>American Mineralogist</i> , 2011 , 96, 437-443	2.9	34
72	Proton dynamics and the phase diagram of dense water ice. <i>Journal of Chemical Physics</i> , 2018 , 148, 214501	9.1	33
71	Influence of NaCl on ice VI and ice VII melting curves up to 6 GPa, implications for large icy moons. <i>Icarus</i> , 2013 , 226, 355-363	3.8	31
70	Raman spectra and lattice dynamics of cubic gauche nitrogen. <i>Journal of Chemical Physics</i> , 2007 , 127, 144510	3.9	31
69	Melt-crystal density crossover in a deep magma ocean. <i>Earth and Planetary Science Letters</i> , 2019 , 516, 202-211	5.3	30
68	Bonding and structural changes in siderite at high pressure. <i>American Mineralogist</i> , 2012 , 97, 1421-1426	2.9	30
67	Theoretical determination of the Raman spectra of MgSiO ₃ perovskite and post-perovskite at high pressure. <i>Geophysical Research Letters</i> , 2006 , 33,	4.9	29
66	The influence of hydrogen on the seismic properties of solid iron. <i>Geophysical Research Letters</i> , 2015 , 42, 3780-3785	4.9	28
65	D/H isotopic fractionation between brucite Mg(OH) ₂ and water from first-principles vibrational modeling. <i>Chemical Geology</i> , 2009 , 262, 159-168	4.2	27
64	Pressure-induced isostructural phase transformation in FeB ₂ . <i>Physical Review B</i> , 2010 , 82,	3.3	26
63	New structures of dense nitrogen: Pathways to the polymeric phase. <i>Chemical Physics Letters</i> , 2007 , 442, 65-70	2.5	26

62	Theoretical determination of the Raman spectra of single-crystal forsterite (Mg ₂ SiO ₄). <i>American Mineralogist</i> , 2010 , 95, 980-986	2.9	25
61	Diamond as a high pressure gauge up to 2.7 Mbar. <i>Applied Physics Letters</i> , 2010 , 97, 251903	3.4	25
60	Stability of phase H in the MgSiO ₃ -H ₂ O-AlOOH-Bi ₂ O ₃ system. <i>Earth and Planetary Science Letters</i> , 2017 , 463, 171-177	5.3	24
59	Salt partitioning between water and high-pressure ices. Implication for the dynamics and habitability of icy moons and water-rich planetary bodies. <i>Earth and Planetary Science Letters</i> , 2017 , 463, 36-47	5.3	24
58	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	2.3	24
57	Synchrotron infrared spectroscopy of the pressure-induced insulator-metal transitions in glassy As ₂ S ₃ and As ₂ Se ₃ . <i>Physical Review B</i> , 2008 , 77,	3.3	24
56	Post-perovskite phase in selected sesquioxides from density-functional calculations. <i>Physical Review B</i> , 2007 , 76,	3.3	23
55	Elasticity and lattice dynamics of enstatite at high pressure. <i>Journal of Geophysical Research: Solid Earth</i> , 2013 , 118, 4071-4082	3.6	22
54	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	2.3	22
53	X-Ray Induced Synthesis of 8H Diamond. <i>Advanced Materials</i> , 2008 , 20, 3303-3307	2.4	22
52	Raman spectroscopy investigation of alpha boron at elevated pressures and temperatures. <i>Solid State Communications</i> , 2013 , 154, 34-39	1.6	20
51	Compressional pathways of cristobalite, structure of cristobalite X-I, and towards the understanding of seifertite formation. <i>Nature Communications</i> , 2017 , 8, 15647	17.4	19
50	Anharmonicity of graphite from UV Raman spectroscopy to 2700 K. <i>Carbon</i> , 2013 , 54, 68-75	10.4	18
49	Ab initio determination of the ground-state properties of Ca ₂ MgSi ₂ O ₇ germanite. <i>Physical Review B</i> , 2003 , 68,	3.3	18
48	Elasticity and dislocations in ice X under pressure. <i>Physics of the Earth and Planetary Interiors</i> , 2014 , 236, 10-15	2.3	17
47	High-pressure compressibility and vibrational properties of (Ca,Mn)CO ₃ . <i>American Mineralogist</i> , 2016 , 101, 2723-2730	2.9	17
46	Carbon sequestration during core formation implied by complex carbon polymerization. <i>Nature Communications</i> , 2019 , 10, 789	17.4	17
45	Serpentines, talc, chlorites, and their high-pressure phase transitions: a Raman spectroscopic study. <i>Physics and Chemistry of Minerals</i> , 2015 , 42, 641-649	1.6	16

44	Prediction of polar ordered oxynitride perovskites. <i>Applied Physics Letters</i> , 2007 , 91, 092902	3.4	15
43	Theoretical determination of the structures of CaSiO ₃ perovskites. <i>Acta Crystallographica Section B: Structural Science</i> , 2006 , 62, 1025-30		15
42	Pressure-induced phase transitions in coesite. <i>American Mineralogist</i> , 2014 , 99, 755-763	2.9	13
41	Is the spin transition in Fe ²⁺ -bearing perovskite visible in seismology?. <i>Geophysical Research Letters</i> , 2010 , 37, n/a-n/a	4.9	12
40	Effect of chemistry on the physical properties of perovskite and post-perovskite. <i>Geophysical Monograph Series</i> , 2007 , 115-128	1.1	12
39	The influence of carbon on the seismic properties of solid iron. <i>Geophysical Research Letters</i> , 2017 , 44, 128-134	4.9	11
38	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	3.6	11
37	High-pressure ferroelastic phase transition in aluminosilicate hollandite. <i>Physical Review B</i> , 2009 , 80,	3.3	11
36	Chemistry and Mineralogy of Earth's Mantle. 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. <i>American Mineralogist</i> , 2014 , 99, 1562-1569	2.9	10
35	Elasticity of AlFeO ₃ and FeAlO ₃ perovskite and post-perovskite from first-principles calculations. <i>Geophysical Research Letters</i> , 2010 , 37, n/a-n/a	4.9	8
34	A database of incommensurate phases. <i>Journal of Applied Crystallography</i> , 2002 , 35, 120-121	3.8	8
33	First-principle study of materials involved in incommensurate transitions. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2005 , 220,	1	8
32	High-pressure behavior of Boron studied on single crystals by X-ray diffraction, Raman and IR spectroscopy. <i>Journal of Solid State Chemistry</i> , 2017 , 245, 50-60	3.3	7
31	Ferroelectricity in high-density H ₂ O ice. <i>Journal of Chemical Physics</i> , 2015 , 142, 134501	3.9	6
30	Anharmonic contribution to the stabilization of Mg(OH) from first principles. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 17799-17808	3.6	6
29	Identifying the spin transition in Fe ²⁺ -rich MgSiO ₃ perovskite from X-ray diffraction and vibrational spectroscopy. <i>American Mineralogist</i> , 2014 , 99, 1270-1276	2.9	6
28	Hydrogen mobility in transition zone silicates. <i>Progress in Earth and Planetary Science</i> , 2017 , 4,	3.9	6
27	Carbon Speciation and Solubility in Silicate Melts. <i>Geophysical Monograph Series</i> , 2020 , 179-194	1.1	5

26	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,	3.9	5
25	Structural, electronic, and dynamical properties of calaverite AuTe ₂ under pressure. <i>Physical Review B</i> , 2004 , 69,	3.3	5
24	Buoyancy and Structure of Volatile-Rich Silicate Melts. <i>Journal of Geophysical Research: Solid Earth</i> , 2021 , 126, e2020JB021045	3.6	5
23	The Critical Point and the Supercritical State of Alkali Feldspars: Implications for the Behavior of the Crust During Impacts. <i>Journal of Geophysical Research E: Planets</i> , 2020 , 125, e2020JE006412	4.1	4
22	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, 633-7		4
21	First-principles study of Pb ₂ MgTeO ₆ : High-T cubic phase and average low-T rhombohedral phase. <i>Physical Review B</i> , 2002 , 65,	3.3	4
20	Crystal Structures of Core Materials. <i>Geophysical Monograph Series</i> , 2016 , 55-68	1.1	4
19	Projector augmented-wave formulation of response to strain and electric-field perturbation within density functional perturbation theory. <i>Physical Review B</i> , 2019 , 99,	3.3	3
18	First-principles determination of the dynamical properties of Pb ₂ MgTeO ₆ . <i>Physical Review B</i> , 2005 , 71,	3.3	3
17	High-pressure yield strength of rocksalt structures using quartz Raman piezometry. <i>Comptes Rendus - Geoscience</i> , 2019 , 351, 71-79	1.4	3
16	Advances in experimental and theoretical isotope geochemistry. <i>Chemical Geology</i> , 2009 , 267, 109-110	4.2	2
15	First-principles study of high-temperature phases of K ₂ SeO ₄ . <i>Physical Review B</i> , 2006 , 74,	3.3	2
14	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	5.3	2
13	Lattice Vibrations and Spectroscopy of Mantle Phases 2015 , 203-231		1
12	Ab Initio Lattice Dynamics and Thermodynamical Properties 2010 , 291-315		1
11	First-principles calculations of K ₂ SeO ₄ dielectrics. <i>AIP Conference Proceedings</i> , 2003 ,	0	1
10	Ab initio study of incommensurately modulated crystals. <i>Computational Materials Science</i> , 2001 , 22, 112-117	3.17	1
9	Theoretical modelling of Raman spectra 173-191		1

8	Stability and Solid Solutions of Hydrous Alumino-Silicates in the Earth's Mantle. <i>Minerals (Basel, Switzerland)</i> , 2020 , 10, 330	2.4	1
7	Analyzing Melts and Fluids from Ab Initio Molecular Dynamics Simulations with the UMD Package. <i>Journal of Visualized Experiments</i> , 2021 ,	1.6	1
6	Stability and spectroscopy of Mg sulfate minerals: Role of hydration on sulfur isotope partitioning. <i>American Mineralogist</i> , 2014 , 99, 1216-1220	2.9	0
5	Genesis of a CO-rich and HO-depleted atmosphere from Earth's early global magma ocean. <i>Science Advances</i> , 2021 , 7, eabj0406	14.3	0
4	High-pressure isosymmetrical phase transition in calaverite. <i>Physics and Chemistry of Minerals</i> , 2004 , 31, 553-558	1.6	
3	First-Principles Calculations of Physical Properties of Planetary Ices. <i>Astrophysics and Space Science Library</i> , 2013 , 149-169	0.3	
2	Gibbs ensemble Monte Carlo simulations of the liquid-vapor equilibrium and the critical point of sodium. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 311-319	3.6	
1	Thermophysical properties of hot fluid iron in the protolunar disk. <i>Physics of the Earth and Planetary Interiors</i> , 2021 , 321, 106806	2.3	