Alberto Garcia

List of Publications by Year
in descending order

72 papers	14,753 citations	117625 34 h-index	95266 68 g-index
74 all docs	74 docs citations	74 times ranked	12323 citing authors

#	Article	IF	Citations
1	The SIESTA method forab initioorder-Nmaterials simulation. Journal of Physics Condensed Matter, 2002, 14, 2745-2779.	1.8	9,150
2	Linear-Scaling ab-initio Calculations for Large and Complex Systems. Physica Status Solidi (B): Basic Research, 1999, 215, 809-817.	1.5	922
3	Finite-Temperature Properties ofPb(Zr1â^'xTix)O3Alloys from First Principles. Physical Review Letters, 2000, 84, 5427-5430.	7.8	568
4	The SIESTA method; developments and applicability. Journal of Physics Condensed Matter, 2008, 20, 064208.	1.8	522
5	Improvements on non-equilibrium and transport Green function techniques: The next-generation transiesta. Computer Physics Communications, 2017, 212, 8-24.	7.5	256
6	First-principles ionicity scales. I. Charge asymmetry in the solid state. Physical Review B, 1993, 47, 4215-4220.	3.2	255
7	Stiff Monatomic Gold Wires with a Spinning Zigzag Geometry. Physical Review Letters, 1999, 83, 3884-3887.	7.8	235
8	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	3.0	229
9	Novel high-pressure structures of MgCO3, CaCO3 and CO2 and their role in Earth's lower mantle. Earth and Planetary Science Letters, 2008, 273, 38-47.	4.4	211
10	Electric-field induced polarization paths inPb(Zr1â^'xTix)O3alloys. Physical Review B, 2001, 64, .	3.2	175
11	Compensation ofp-Type Doping in ZnSe: The Role of Impurity-Native Defect Complexes. Physical Review Letters, 1995, 74, 1131-1134.	7.8	172
12	Use of gradient-corrected functionals in total-energy calculations for solids. Physical Review B, 1992, 46, 9829-9832.	3.2	126
13	Electromechanical behavior of BaTiO3 from first principles. Applied Physics Letters, 1998, 72, 2981-2983.	3.3	113
14	Competing structural instabilities in the ferroelectric Aurivillius compoundSrBi2Ta2O9. Physical Review B, 2004, 70, .	3.2	104
15	Optimal strictly localized basis sets for noble metal surfaces. Physical Review B, 2009, 79, .	3.2	100
16	First-principles study of Zn- and Se-stabilized ZnSe(100) surface reconstructions. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1994, 12, 2678.	1.6	99
17	Low-Temperature Properties of Pb(Zr 1â^' x Ti x)O 3 Solid Solutions near the Morphotropic Phase Boundary. Ferroelectrics, 2002, 266, 41-56.	0.6	95
18	First-principles study of stability and vibrational properties of tetragonalPbTiO3. Physical Review B, 1996, 54, 3817-3824.	3.2	93

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19	First-principles prediction of high-temperature superconductivity in metallic hydrogen. Nature, 1989, 340, 369-371.	27.8	80
20	ELSI: A unified software interface for Kohnâ€“Sham electronic structure solvers. Computer Physics Communications, 2018, 222, 267-285.	7.5	78
21	Stress relief from alternately buckled dimers in Si(100). Physical Review B, 1993, 48, 17350-17353.	3.2	58
22	Quasiparticle spectra of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>2</mml:mn><mml:mi>H</mml:mi><mml:mo>-</mml:mo><mml:m Two-band superconductivity and the role of tunneling selectivity. Physical Review B, 2015, 92, .	3.2	56
23	Band Gap Closure and Metallization of Molecular Solid Hydrogen. Europhysics Letters, 1990, 13, 355-360.	2.0	54
24	Multiple instabilities in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Bi</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">Ti</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>12</mml:mn></mml:msub></mml:mrow></mml:math>: A ferroelectric beyond the soft-mode paradigm. Physical Review B, 2008, 77, .	3.2	53
25	Devonshire-Landau free energy ofBaTiO3from first principles. Physical Review B, 2001, 63, .	3.2	50
26	Two distinct metallic bands associated with monatomic Au wires on the Si(557)-Au surface. Physical Review B, 2002, 65, .	3.2	48
27	Dependence of the lone pair of bismuth on coordination environment and pressure: An ab initio study on Cu4Bi5S10 and Bi2S3. Journal of Solid State Chemistry, 2010, 183, 2133-2143.	2.9	47
28	Phosphine adsorption and decomposition on Si(100) 2Ã—1 studied by STM. Physical Review B, 1995, 52, 5843-5850.	3.2	46
29	First-principles ionicity scales. II. Structural coordinates from atomic calculations. Physical Review B, 1993, 47, 4221-4225.	3.2	45
30	Calculation of core level shifts within DFT using pseudopotentials and localized basis sets. European Physical Journal B, 2012, 85, 1.	1.5	44
31	Ultrahigh-Pressure Melting of Lead: A Multidisciplinary Study. Science, 1990, 248, 462-465.	12.6	43
32	Large Induced Interface Dipole Moments without Charge Transfer: Buckybowls on Metal Surfaces. Journal of Physical Chemistry Letters, 2011, 2, 2805-2809.	4.6	43
33	The structure and dynamics of crystalline durene by neutron scattering and numerical modelling using density functional methods. Chemical Physics, 2000, 261, 189-203.	1.9	39
34	The psml format and library for norm-conserving pseudopotential data curation and interoperability. Computer Physics Communications, 2018, 227, 51-71.	7.5	38
35	Hybrid DNA-gold nanostructured materials: anab initioapproach. Nanotechnology, 2001, 12, 126-131.	2.6	35
36	Linear-Scaling ab-initio Calculations for Large and Complex Systems. , 1999, 215, 809.		35

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37	An efficient implementation of a QMâ€“MM method in SIESTA. Theoretical Chemistry Accounts, 2011, 128, 825-833.	1.4	29
38	Seâ€rich phase of ZnSe(100) predicted by totalâ€energy calculations. Applied Physics Letters, 1994, 65, 708-710.	3.3	28
39	ELSI â€" An open infrastructure for electronic structure solvers. Computer Physics Communications, 2020, 256, 107459.	7.5	27
40	Comparison of empirical bond-valence and first-principles energy calculations for a complex structural instability. Physical Review B, 2005, 72, .	3.2	26
41	SIESTA-PEXSI: massively parallel method for efficient and accurateab initiomaterials simulation without matrix diagonalization. Journal of Physics Condensed Matter, 2014, 26, 305503.	1.8	25
42	Selfâ€Organized Ce_{1â€x}Gd_xO_{2â€y} Nanowire Networks with Very Fast Coarsening Driven by Attractive Elastic Interactions. Small, 2010, 6, 2716-2724.	10.0	22
43	Revision of pyrrhotite structures within a common superspace model. Acta Crystallographica Section B: Structural Science, 2007, 63, 693-702.	1.8	21
44	Theoretical Investigation of the Binding Process of Corannulene on a Cu(111) Surface^{â€}. Journal of Physical Chemistry A, 2010, 114, 8864-8872.	2.5	21
45	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
46	Dielectric properties of solid molecular hydrogen at high pressure. Physical Review B, 1992, 45, 9709-9715.	3.2	16
47	Atomic rearrangement at the interface of annealed ZnSe films grown on vicinal Si(001) substrates. Physical Review B, 1994, 50, 4416-4423.	3.2	16
48	Interplay between theory and experiment in solid state inorganic chemistry. Journal of Materials Chemistry, 2001, 11, 1-10.	6.7	15
49	First-principles study of the ferroelastic phase transition inCaCl2. Physical Review B, 2002, 65, .	3.2	15
50	Displacive vs. order-disorder in structural phase transitions. Ferroelectrics, 2000, 236, 93-103.	0.6	12
51	Thermodynamic stability analysis of isometric and elongated epitaxial<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ce</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn> Physical Review B, 2010, 82, .	3.2	11
52	Implementation of non-collinear spin-constrained DFT calculations in SIESTA with a fully relativistic Hamiltonian. JPhys Materials, 2018, 1, 015010.	4.2	11
53	Optimized local modes for lattice-dynamical applications. Physical Review B, 2000, 61, 3127-3130.	3.2	10
54	Superlattice pseudouniform orderings as modulated structures: Stripe and checkerboard arrangements. Physical Review B, 2011, 84, .	3.2	10

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55	Aluminum ordering and clustering in Al-rich synthetic phlogopite: Â -> 29Si CPMAS HETCOR spectroscopy and atomistic calculations. American Mineralogist, 2012, 97, 341-352.	1.9	10
56	Common workflows for computing material properties using different quantum engines. Npj Computational Materials, 2021, 7, .	8.7	10
57	Dynamics of incommensurate structures and inelastic neutron scattering. Physical Review B, 1989, 39, 2476-2483.	3.2	9
58	CML tools and information flow in atomic scale simulations. Molecular Simulation, 2005, 31, 315-322.	2.0	9
59	An efficient computational method for use in structural studies of crystals with substitutional disorder. Journal of Physics Condensed Matter, 2010, 22, 415401.	1.8	9
60	Validity of the on-site spin-orbit coupling approximation. Physical Review B, 2021, 104, .	3.2	9
61	Crystal structure determination of karibibite, an Fe3+ arsenite, using electron diffraction tomography. Mineralogical Magazine, 2017, 81, 1191-1202.	1.4	8
62	Analysis of soft optical modes in hexagonal BaTiO3: transference of perovskite local distortions. Journal of Physics Condensed Matter, 2000, 12, L387-L391.	1.8	6
63	Electronic Structure of the A₈Tr₁₁ (A = K, Rb, Cs; Tr = Ga, In, Tl) Zintl Phases: Possible Chemical Reasons Behind Their Activated versus Non Activated Conductivity. Inorganic Chemistry, 2009, 48, 9792-9799.	4.0	6
64	Charge Delocalization, Oxidation States, and Silver Mobility in the Mixed Silverâ€“Copper Oxide AgCuO₂. Inorganic Chemistry, 2019, 58, 7026-7035.	4.0	5
65	First-principles study of ferroelasticity in CaCl2and As2O5. Ferroelectrics, 2000, 237, 73-80.	0.6	4
66	Ag2Cu3Cr2O8(OH)4: a new bidimensional silverâ€“copper mixed-oxyhydroxide with in-plane ferromagnetic coupling. Dalton Transactions, 2017, 46, 1093-1104.	3.3	4
67	Electronic Structure Calculations with Localized Orbitals: The Siesta Method. , 2005, , 77-91.		3
68	First-principles study of the structural instabilities in hexagonal barium titanate: Coupling between the soft optical and the acoustic Modes. Ferroelectrics, 2000, 237, 25-32.	0.6	2
69	Compositional uniformity, domain patterning and the mechanism underlying nano-chessboard arrays. Journal of Physics Condensed Matter, 2012, 24, 495301.	1.8	2
70	Theoretical Study of a new Transition Sequence in III-V Compounds: High-Pressure Phases of InSb. Materials Research Society Symposia Proceedings, 1990, 193, 89.	0.1	0
71	Theoretical Study of High Pressure Metallic Hydrogen. Materials Research Society Symposia Proceedings, 1990, 193, 15.	0.1	0
72	Linear phonon-strain coupling in structural phase transitions: Stability of tetragonal PbTiO3. Ferroelectrics, 1997, 194, 29-38.	0.6	0