Alberto Garcia

List of Publications by Year
in descending order

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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	Common workflows for computing material properties using different quantum engines. Npj Computational Materials, 2021, 7, .	8.7	10
2	Validity of the on-site spin-orbit coupling approximation. Physical Review B, 2021, 104, .	3.2	9
3	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
4	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	3.0	229
5	ELSI â€” An open infrastructure for electronic structure solvers. Computer Physics Communications, 2020, 256, 107459.	7.5	27
6	Charge Delocalization, Oxidation States, and Silver Mobility in the Mixed Silverâ€"Copper Oxide AgCuO₂. Inorganic Chemistry, 2019, 58, 7026-7035.	4.0	5
7	The psml format and library for norm-conserving pseudopotential data curation and interoperability. Computer Physics Communications, 2018, 227, 51-71.	7.5	38
8	ELSI: A unified software interface for Kohnâ€"Sham electronic structure solvers. Computer Physics Communications, 2018, 222, 267-285.	7.5	78
9	Implementation of non-collinear spin-constrained DFT calculations in SIESTA with a fully relativistic Hamiltonian. JPhys Materials, 2018, 1, 015010.	4.2	11
10	Ag2Cu3Cr2O8(OH)4: a new bidimensional silverâ€"copper mixed-oxyhydroxide with in-plane ferromagnetic coupling. Dalton Transactions, 2017, 46, 1093-1104.	3.3	4
11	Improvements on non-equilibrium and transport Green function techniques: The next-generation transiesta. Computer Physics Communications, 2017, 212, 8-24.	7.5	256
12	Crystal structure determination of karibibite, an Fe3+ arsenite, using electron diffraction tomography. Mineralogical Magazine, 2017, 81, 1191-1202.	1.4	8
13	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>â€'</mm Two-band superconductivity and the role of tunneling selectivity. Physical Review B, 2015, 92, .	3.2	56
14	SIESTA-PEXSI: massively parallel method for efficient and accurate<i>ab initio</i>materials simulation without matrix diagonalization. Journal of Physics Condensed Matter, 2014, 26, 305503.	1.8	25
15	Compositional uniformity, domain patterning and the mechanism underlying nano-chessboard arrays. Journal of Physics Condensed Matter, 2012, 24, 495301.	1.8	2
16	Calculation of core level shifts within DFT using pseudopotentials and localized basis sets. European Physical Journal B, 2012, 85, 1.	1.5	44
17	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
18	Large Induced Interface Dipole Moments without Charge Transfer: Buckybowls on Metal Surfaces. Journal of Physical Chemistry Letters, 2011, 2, 2805-2809.	4.6	43

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19	Superlattice pseudouniform orderings as modulated structures: Stripe and checkerboard arrangements. Physical Review B, 2011, 84, .	3.2	10
20	An efficient implementation of a QMâ€“MM method in SIESTA. Theoretical Chemistry Accounts, 2011, 128, 825-833.	1.4	29
21	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
22	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
23	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
24	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
25	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
26	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
27	Optimal strictly localized basis sets for noble metal surfaces. Physical Review B, 2009, 79, .	3.2	100
28	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
29	The SIESTA method; developments and applicability. Journal of Physics Condensed Matter, 2008, 20, 064208.	1.8	522
30	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: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
31	Revision of pyrrhotite structures within a common superspace model. Acta Crystallographica Section B: Structural Science, 2007, 63, 693-702.	1.8	21
32	Electronic Structure Calculations with Localized Orbitals: The Siesta Method. , 2005, , 77-91.		3
33	Comparison of empirical bond-valence and first-principles energy calculations for a complex structural instability. Physical Review B, 2005, 72, .	3.2	26
34	CML tools and information flow in atomic scale simulations. Molecular Simulation, 2005, 31, 315-322.	2.0	9
35	Competing structural instabilities in the ferroelectric Aurivillius compoundSrBi2Ta2O9. Physical Review B, 2004, 70, .	3.2	104
36	First-principles study of the ferroelastic phase transition inCaCl2. Physical Review B, 2002, 65, .	3.2	15

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37	Two distinct metallic bands associated with monatomic Au wires on the Si(557)-Au surface. Physical Review B, 2002, 65, .	3.2	48
38	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
39	The SIESTA method forab initioorder-Nmaterials simulation. Journal of Physics Condensed Matter, 2002, 14, 2745-2779.	1.8	9,150
40	Electric-field induced polarization paths inPb(Zr1â^'xTix)O3alloys. Physical Review B, 2001, 64, .	3.2	175
41	Interplay between theory and experiment in solid state inorganic chemistry. Journal of Materials Chemistry, 2001, 11, 1-10.	6.7	15
42	Devonshire-Landau free energy ofBaTiO3from first principles. Physical Review B, 2001, 63, .	3.2	50
43	Hybrid DNA-gold nanostructured materials: anab initioapproach. Nanotechnology, 2001, 12, 126-131.	2.6	35
44	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
45	Optimized local modes for lattice-dynamical applications. Physical Review B, 2000, 61, 3127-3130.	3.2	10
46	Displacive vs. order-disorder in structural phase transitions. Ferroelectrics, 2000, 236, 93-103.	0.6	12
47	Finite-Temperature Properties ofPb(Zr1â^'xTix)O3Alloys from First Principles. Physical Review Letters, 2000, 84, 5427-5430.	7.8	568
48	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
49	First-principles study of ferroelasticity in CaCl2and As2O5. Ferroelectrics, 2000, 237, 73-80.	0.6	4
50	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
51	Stiff Monatomic Gold Wires with a Spinning Zigzag Geometry. Physical Review Letters, 1999, 83, 3884-3887.	7.8	235
52	Linear-Scaling ab-initio Calculations for Large and Complex Systems. Physica Status Solidi (B): Basic Research, 1999, 215, 809-817.	1.5	922
53	Linear-Scaling ab-initio Calculations for Large and Complex Systems. , 1999, 215, 809.		35
54	Electromechanical behavior of BaTiO3 from first principles. Applied Physics Letters, 1998, 72, 2981-2983.	3.3	113

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55	Linear phonon-strain coupling in structural phase transitions: Stability of tetragonal PbTiO3. Ferroelectrics, 1997, 194, 29-38.	0.6	0
56	First-principles study of stability and vibrational properties of tetragonalPbTiO3. Physical Review B, 1996, 54, 3817-3824.	3.2	93
57	Phosphine adsorption and decomposition on Si(100) 2Ã—1 studied by STM. Physical Review B, 1995, 52, 5843-5850.	3.2	46
58	Compensation ofp-Type Doping in ZnSe: The Role of Impurity-Native Defect Complexes. Physical Review Letters, 1995, 74, 1131-1134.	7.8	172
59	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
60	Seâ€rich phase of ZnSe(100) predicted by totalâ€energy calculations. Applied Physics Letters, 1994, 65, 708-710.	3.3	28
61	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
62	Stress relief from alternately buckled dimers in Si(100). Physical Review B, 1993, 48, 17350-17353.	3.2	58
63	First-principles ionicity scales. I. Charge asymmetry in the solid state. Physical Review B, 1993, 47, 4215-4220.	3.2	255
64	First-principles ionicity scales. II. Structural coordinates from atomic calculations. Physical Review B, 1993, 47, 4221-4225.	3.2	45
65	Dielectric properties of solid molecular hydrogen at high pressure. Physical Review B, 1992, 45, 9709-9715.	3.2	16
66	Use of gradient-corrected functionals in total-energy calculations for solids. Physical Review B, 1992, 46, 9829-9832.	3.2	126
67	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
68	Theoretical Study of High Pressure Metallic Hydrogen. Materials Research Society Symposia Proceedings, 1990, 193, 15.	0.1	0
69	Band Gap Closure and Metallization of Molecular Solid Hydrogen. Europhysics Letters, 1990, 13, 355-360.	2.0	54
70	Ultrahigh-Pressure Melting of Lead: A Multidisciplinary Study. Science, 1990, 248, 462-465.	12.6	43
71	First-principles prediction of high-temperature superconductivity in metallic hydrogen. Nature, 1989, 340, 369-371.	27.8	80
72	Dynamics of incommensurate structures and inelastic neutron scattering. Physical Review B, 1989, 39, 2476-2483.	3.2	9