Xavier Gonze

List of Publications by Year
in descending order

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108	20,622	53794 45	24982 109
papers	citations	h-index	g-index

110	110	110	14585
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	First-principles computation of material properties: the ABINIT software project. Computational Materials Science, 2002, 25, 478-492.	3.0	2,789
2	Dynamical matrices, Born effective charges, dielectric permittivity tensors, and interatomic force constants from density-functional perturbation theory. Physical Review B, 1997, 55, 10355-10368.	3.2	2,534
3	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	7.5	2,297
4	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
5	A brief introduction to the ABINIT software package. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	1,101
6	The PseudoDojo: Training and grading a 85 element optimized norm-conserving pseudopotential table. Computer Physics Communications, 2018, 226, 39-54.	7.5	1,001
7	First-principles responses of solids to atomic displacements and homogeneous electric fields: Implementation of a conjugate-gradient algorithm. Physical Review B, 1997, 55, 10337-10354.	3.2	920
8	Recent developments in the ABINIT software package. Computer Physics Communications, 2016, 205, 106-131.	7.5	662
9	Adiabatic density-functional perturbation theory. Physical Review A, 1995, 52, 1096-1114.	2.5	539
10	Identification and design principles of low hole effective mass p-type transparent conducting oxides. Nature Communications, 2013, 4, 2292.	12.8	507
11	Implementation of the projector augmented-wave method in the ABINIT code: Application to the study of iron under pressure. Computational Materials Science, 2008, 42, 337-351.	3.0	484
12	Dynamical atomic charges: The case ofABO3compounds. Physical Review B, 1998, 58, 6224-6240.	3.2	482
13	Dielectric tensor, effective charges, and phonons in Î±-quartz by variational density-functional perturbation theory. Physical Review Letters, 1992, 68, 3603-3606.	7.8	436
14	Density-functional approach to nonlinear-response coefficients of solids. Physical Review B, 1989, 39, 13120-13128.	3.2	382
15	The Abinitproject: Impact, environment and recent developments. Computer Physics Communications, 2020, 248, 107042.	7.5	369
16	Ab initiocalculation of the thermodynamic properties and atomic temperature factors ofSiO2Î±-quartz and stishovite. Physical Review B, 1995, 51, 8610-8613.	3.2	287
17	Density-Polarization Functional Theory of the Response of a Periodic Insulating Solid to an Electric Field. Physical Review Letters, 1995, 74, 4035-4038.	7.8	275
18	Incipient Metals: Functional Materials with a Unique Bonding Mechanism. Advanced Materials, 2018, 30, e1803777.	21.0	255

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19	Nonlinear optical susceptibilities, Raman efficiencies, and electro-optic tensors from first-principles density functional perturbation theory. Physical Review B, 2005, 71, .	3.2	243
20	Berry-phase treatment of the homogeneous electric field perturbation in insulators. Physical Review B, 2001, 63, .	3.2	240
21	Accurate<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>self-energies in a plane-wave basis using only a few empty states: Towards large systems. Physical Review B, 2008, 78, .	3.2	194
22	ABINIT: Overview and focus on selected capabilities. Journal of Chemical Physics, 2020, 152, 124102.	3.0	179
23	Many-Body Effects on the Zero-Point Renormalization of the Band Structure. Physical Review Letters, 2014, 112, .	7.8	141
24	Temperature dependence of the electronic structure of semiconductors and insulators. Journal of Chemical Physics, 2015, 143, 102813.	3.0	139
25	How Does Chemistry Influence Electron Effective Mass in Oxides? A High-Throughput Computational Analysis. Chemistry of Materials, 2014, 26, 5447-5458.	6.7	127
26	Band widths and gaps from the Tran-Blaha functional: Comparison with many-body perturbation theory. Physical Review B, 2013, 87, .	3.2	125
27	High-throughput density-functional perturbation theory phonons for inorganic materials. Scientific Data, 2018, 5, 180065.	5.3	122
28	High-Mobility Bismuth-based Transparent p-Type Oxide from High-Throughput Material Screening. Chemistry of Materials, 2016, 28, 30-34.	6.7	118
29	Atypical Excitonâ€“Phonon Interactions in WS₂ and WSe₂ Monolayers Revealed by Resonance Raman Spectroscopy. Nano Letters, 2016, 16, 2363-2368.	9.1	118
30	Statistical Analysis of Coordination Environments in Oxides. Chemistry of Materials, 2017, 29, 8346-8360.	6.7	115
31	First-Principles Study of the Electro-Optic Effect in Ferroelectric Oxides. Physical Review Letters, 2004, 93, 187401.	7.8	108
32	Dynamical and anharmonic effects on the electron-phonon coupling and the zero-point renormalization of the electronic structure. Physical Review B, 2015, 92, .	3.2	104
33	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msup><mml:msup><mml:mi>W</mml:mi> gap of ZnO: Effects of plasmon-pole models. Physical Review B, 2011, 84, .	3.2	101
34	Temperature dependence of electronic eigenenergies in the adiabatic harmonic approximation. Physical Review B, 2014, 90, .	3.2	91
35	Verification of first-principles codes: Comparison of total energies, phonon frequencies, electronâ€“phonon coupling and zero-point motion correction to the gap between ABINIT and QE/Yambo. Computational Materials Science, 2014, 83, 341-348.	3.0	88
36	Theoretical approaches to the temperature and zeroâ€point motion effects on the electronic band structure. Annalen Der Physik, 2011, 523, 168-178.	2.4	81

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37	Abinitiostudy of the volume dependence of dynamical and thermodynamical properties of silicon. Physical Review B, 1996, 53, 4488-4497.	3.2	76
38	First-principle studies of the lattice dynamics of crystals, and related properties. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	72
39	Density functional perturbation theory with spin-orbit coupling: Phonon band structure of lead. Physical Review B, 2008, 78, .	3.2	66
40	Predominance of non-adiabatic effects in zero-point renormalization of the electronic band gap. Npj Computational Materials, 2020, 6, .	8.7	65
41	Quasiparticles and phonon satellites in spectral functions of semiconductors and insulators: Cumulants applied to the full first-principles theory and the FrÃ¶hlich polaron. Physical Review B, 2018, 97, .	3.2	60
42	Electron-Phonon beyond FrÃ¶hlich: Dynamical Quadrupoles in Polar and Covalent Solids. Physical Review Letters, 2020, 125, 136601.	7.8	60
43	Understanding Thermal Quenching of Photoluminescence in Oxynitride Phosphors from First Principles. Journal of Physical Chemistry C, 2016, 120, 4040-4047.	3.1	58
44	Interatomic force constants including the DFT-D dispersion contribution. Physical Review B, 2016, 93, .	3.2	50
45	First-principles study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msup><mml:mrow><mml:mi>Ce</mml:mi></mml:mrow><mml silicate nitride phosphors: Neutral excitation, Stokes shift, and luminescent center identification. Physical Review B, 2016, 93, .	3.2	49
46	Phonon-limited electron mobility in Si, GaAs, and GaP with exact treatment of dynamical quadrupoles. Physical Review B, 2020, 102, .	3.2	47
47	Many-body perturbation theory approach to the electron-phonon interaction with density-functional theory as a starting point. Physical Review B, 2015, 91, .	3.2	46
48	Automation methodologies and large-scale validation for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m : Towards high-throughput <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m calculations. Physical Review B, 2017, 96, .	3.2	45
49	First-principles study of the luminescence of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>Eu</mml:mi></mml:mrow><mml:mrow><mml -doped phosphors. Physical Review B, 2017, 96, .	3.2	44
50	First-principles thermodynamical properties of semiconductors. Physical Review Letters, 1990, 64, 2961-2961.	7.8	39
51	Casting Light on the Darkening of Colors in Historical Paintings. Physical Review Letters, 2013, 111, 208302.	7.8	38
52	Implementation and testing of Lanczos-based algorithms for Random-Phase Approximation eigenproblems. Computational Materials Science, 2011, 50, 2148-2156.	3.0	37
53	Projector augmented-wave approach to density-functional perturbation theory. Physical Review B, 2006, 73, .	3.2	35
54	Assessment of Firstâ€Principles and Semiempirical Methodologies for Absorption and Emission Energies of Ce³⁺â€Doped Luminescent Materials. Advanced Optical Materials, 2017, 5, 1600997.	7.3	35

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55	Origin of the counterintuitive dynamic charge in the transition metal dichalcogenides. Physical Review B, 2017, 95, .	3.2	34
56	First-principles study of excitonic effects in Raman intensities. Physical Review B, 2013, 88, .	3.2	33
57	Density-operator theory of orbital magnetic susceptibility in periodic insulators. Physical Review B, 2011, 84, .	3.2	30
58	Preconditioning of self-consistent-field cycles in density-functional theory: The extrapolar method. Physical Review B, 2008, 78, .	3.2	29
59	Precise effective masses from density functional perturbation theory. Physical Review B, 2016, 93, .	3.2	28
60	Ab Initio Approach to Second-order Resonant Raman Scattering Including Exciton-Phonon Interaction. Scientific Reports, 2017, 7, 7344.	3.3	27
61	Band gap renormalization, carrier mobilities, and the electron-phonon self-energy in crystalline naphthalene. Physical Review B, 2020, 101, .	3.2	26
62	Consistent treatment of charged systems within periodic boundary conditions: The projector augmented-wave and pseudopotential methods revisited. Physical Review B, 2014, 89, .	3.2	25
63	Vibrational and dielectric properties of the bulk transition metal dichalcogenides. Physical Review Materials, 2018, 2, .	2.4	25
64	Effects of plasmon pole models on the G0W0 electronic structure of various oxides. European Physical Journal B, 2012, 85, 1.	1.5	24
65	The ETSF: An e-Infrastructure That Bridges Simulations and Experiments. Computing in Science and Engineering, 2012, 14, 22-32.	1.2	24
66	Origin of Magnetism and Quasiparticles Properties in Cr-Doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2013, 110, 136402.	7.8	24
67	First-principles investigation of the structural, dynamical, and dielectric properties of kesterite, stannite, and PMCA phases of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2016, 94, .	3.2	23
68	Photoelasticity ofÎ±-quartz from first principles. Physical Review B, 2001, 63, .	3.2	22
69	Time-dependent density functional theory study of charge transfer in collisions. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	21
70	ChemEnv: a fast and robust coordination environment identification tool. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 683-695.	1.1	21
71	Phonon band structure and electron-phonon interactions in metallic nanowires. Physical Review B, 2006, 74, .	3.2	20
72	Convergence of quasiparticle band structures of Si and Ge nanowires in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="italic">GW</mml:mi></mml:mrow></mml:math>approximation and the validity of scissor shifts. Physical Review B, 2011, 83, .	3.2	20

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73	Computed electronic and optical properties of SnO2 under compressive stress. Optical Materials, 2014, 38, 161-166.	3.6	20
74	Temperature evolution of the band gap in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub></m by resonant Raman scattering. Physical Review B, 2016, 93, .	3.2	20
75	Convergence and pitfalls of density functional perturbation theory phonons calculations from a high-throughput perspective. Computational Materials Science, 2018, 144, 331-337.	3.0	19
76	Theoretical Approach for White-LED Phosphors: from Crystal Structures to Optical Properties. IOP Conference Series: Materials Science and Engineering, 2011, 18, 102001.	0.6	18
77	Computational Modeling of 2D Materials under High Pressure and Their Chemical Bonding: Silicene as Possible Field-Effect Transistor. ACS Nano, 2021, 15, 6861-6871.	14.6	18
78	Finite homogeneous electric fields in the projector augmented wave formalism: Applications to linear and nonlinear response. Computational Materials Science, 2012, 58, 113-118.	3.0	16
79	Ab initio study of luminescence in Ce-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Lu</mml:mi><mml:mn>2</mml:mn></mml:m : The role of oxygen vacancies on emission color and thermal quenching behavior. Physical Review	2.4	16
80	First-principles study of paraelectric and ferroelectric<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">CsH</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">PO</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>including dispersion forces: Stability and related vibrational, dielectric, and elastic properties. Physical Review B, 2017, 95, .	3.2	15
81	Comparison between projector augmented-wave and ultrasoft pseudopotential formalisms at the density-functional perturbation theory level. Physical Review B, 2008, 78, .	3.2	14
82	Implementation of techniques for computing optical properties in 0â€“3 dimensions, including a real-space cutoff, in ABINIT. Computational Materials Science, 2010, 50, 698-703.	3.0	13
83	First-principles and experimental characterization of the electronic and optical properties of CaS and CaO. Optical Materials, 2013, 35, 1477-1480.	3.6	13
84	First-principles characterization of the electronic and optical properties of hexagonal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si79.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">LiIO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml Optical Materials, 2014, 36, 1494-1501.	3.6	13
85	Ab-initio study of oxygen vacancy stability in bulk and Cerium-doped lutetium oxyorthosilicate. Journal of Luminescence, 2018, 204, 499-505.	3.1	13
86	Variations on the â€œexact factorizationâ€•theme. European Physical Journal B, 2018, 91, 1.	1.5	11
87	Large phosphorene in-plane contraction induced by interlayer interactions in graphene-phosphorene heterostructures. Physical Review Materials, 2018, 2, .	2.4	11
88	Efficient on-the-fly interpolation technique for Betheâ€“Salpeter calculations of optical spectra. Computer Physics Communications, 2016, 203, 83-93.	7.5	10
89	Beyond the one-dimensional configuration coordinate model of photoluminescence. Physical Review B, 2019, 100, .	3.2	10
90	Importance of Longâ€•Range Channel Sr Displacements for the Narrow Emission in Sr[Li₂Al₂O₂N₂]:Eu²⁺Phosphor. Advanced Optical Materials, 2021, 9, 2100649.	7.3	10

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91	Vibrational and dielectric properties of monolayer transition metal dichalcogenides. Physical Review Materials, 2019, 3, .	2.4	10
92	Srâ€Doped Superionic Hydrogen Glass: Synthesis and Properties of SrH₂₂. Advanced Materials, 2022, 34, e2200924.	21.0	10
93	Sharing electronic structure and crystallographic data with ETSF_IO. Computer Physics Communications, 2008, 179, 748-758.	7.5	9
94	First-principle study of materials involved in incommensurate transitions. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	8
95	Quasiparticle electronic structure of barium-silicon oxynitrides for white-LED application. Physical Review B, 2013, 88, .	3.2	8
96	FrÃ¶hlich polaron effective mass and localization length in cubic materials: Degenerate and anisotropic electronic bands. Physical Review B, 2021, 104, .	3.2	8
97	Pseudopotentials Plane Waves?Projector Augmented Waves: A Primer. Physica Scripta, 2004, T109, 40.	2.5	7
98	Specification of an extensible and portable file format for electronic structure and crystallographic data. Computational Materials Science, 2008, 43, 1056-1065.	3.0	7
99	Structural, electronic, vibrational, and dielectric properties of LaBGeO5 from first principles. Journal of Applied Physics, 2014, 115, 074103.	2.5	7
100	Band gap bowing and spectral width of Ga<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e895" altimg="si105.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi><mml:mo>)</ xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e912" altimg="si106.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mi>x</mml:mi></mml:mrow></mml:ms	2.7	6
101	â€œSelf-trappingâ€in solar cell hybrid inorganic-organic perovskite absorbers. Applied Materials Today, 2022, 26, 101380.	4.3	6
102	Wannier functions approach to van der Waals interactions in ABINIT. Computer Physics Communications, 2012, 183, 480-485.	7.5	5
103	Variational polaron equationsÂapplied to the anisotropic FrÃ¶hlich model. Physical Review B, 2022, 105, .	3.2	5
104	Spinâ€“orbit effects in the bismuth atom and dimer: tight-binding and density functional theory comparison. Journal of Physics B: Atomic, Molecular and Optical Physics, 2013, 46, 095101.	1.5	4
105	First-principles investigation of CZTS Raman spectra. Physical Review Materials, 2022, 6, .	2.4	4
106	Spectroscopic signatures of nonpolarons: the case of diamond. Physical Chemistry Chemical Physics, 2022, 24, 12580-12591.	2.8	4
107	Li diffusion in Si and LiSi: Nuclear quantum effects and anharmonicity. Journal of Chemical Physics, 2020, 152, 244101.	3.0	2
108	Accurate quantumâ€“mechanical evaluation of the electric polarization of periodic solids using a multi-step method. Computational Materials Science, 2012, 63, 312-318.	3.0	1