Paolo Giannozzi

List of Publications by Year
in descending order

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113 papers	40,766 citations	81900 39 h-index	34986 98 g-index
114 all docs	114 docs citations	114 times ranked	30677 citing authors

#	Article	IF	Citations
1	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	1.8	18,183
2	Phonons and related crystal properties from density-functional perturbation theory. Reviews of Modern Physics, 2001, 73, 515-562.	45.6	7,534
3	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
4	Greenâ€™s-function approach to linear response in solids. Physical Review Letters, 1987, 58, 1861-1864.	7.8	1,807
5	Ab initiocalculation of phonon dispersions in semiconductors. Physical Review B, 1991, 43, 7231-7242.	3.2	1,619
6	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
7	Q<scp>uantum</scp> ESPRESSO toward the exascale. Journal of Chemical Physics, 2020, 152, 154105.	3.0	796
8	Gas adsorption on graphene doped with B, N, Al, and S: A theoretical study. Applied Physics Letters, 2009, 95, .	3.3	643
9	Ab initiolattice dynamics of diamond. Physical Review B, 1993, 48, 3156-3163.	3.2	298
10	Density-Functional Perturbation Theory for Quasi-Harmonic Calculations. Reviews in Mineralogy and Geochemistry, 2010, 71, 39-57.	4.8	265
11	Oxygen adsorption on graphite and nanotubes. Journal of Chemical Physics, 2003, 118, 1003-1006.	3.0	261
12	Coverage-Dependent Adsorption of CH3S and (CH3S)2on Au(111):Â a Density Functional Theory Study. Journal of Physical Chemistry B, 2001, 105, 9509-9513.	2.6	230
13	Reaction Pathways for Oxygen Evolution Promoted by Cobalt Catalyst. Journal of the American Chemical Society, 2013, 135, 15353-15363.	13.7	228
14	Vibrational and dielectric properties of C60 from densityâ€functional perturbation theory. Journal of Chemical Physics, 1994, 100, 8537-8539.	3.0	184
15	First-principles codes for computational crystallography in the Quantum-ESPRESSO package. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.8	177
16	Structure and thermodynamics ofSixGe1â^'xalloys fromab initioMonte Carlo simulations. Physical Review Letters, 1991, 66, 2116-2119.	7.8	155
17	Towards Very Large-Scale Electronic-Structure Calculations. Europhysics Letters, 1992, 17, 547-552.	2.0	155
18	Calculation of near-edge x-ray-absorption fine structure at finite temperatures: Spectral signatures of hydrogen bond breaking in liquid water. Journal of Chemical Physics, 2004, 120, 8632-8637.	3.0	148

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19	Thirteenâ€atom clusters: Equilibrium geometries, structural transformations, and trends in Na, Mg, Al, and Si. Journal of Chemical Physics, 1992, 96, 1248-1256.	3.0	140
20	Phonon spectra of ultrathin GaAs/AlAs superlattices: Anab initiocalculation. Physical Review B, 1990, 41, 3870-3873.	3.2	116
21	Phonon dispersions inGaxAl1â^'xAs alloys. Physical Review Letters, 1990, 65, 84-87.	7.8	108
22	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	3.3	108
23	First-principle molecular dynamics with ultrasoft pseudopotentials: Parallel implementation and application to extended bioinorganic systems. Journal of Chemical Physics, 2004, 120, 5903-5915.	3.0	95
24	Second-order Raman spectra of diamond fromab initiophonon calculations. Physical Review B, 1993, 48, 3164-3170.	3.2	94
25	Structure and bonding in cisplatin and other Pt(II) complexes. Chemical Physics Letters, 1995, 234, 50-56.	2.6	91
26	Atomic and molecular hydrogen in gallium arsenide: A theoretical study. Physical Review B, 1992, 46, 4621-4629.	3.2	89
27	Effects of disorder on the Raman spectra of GaAs/AlAs superlattices. Physical Review B, 1992, 45, 4280-4288.	3.2	88
28	Elastic Constants of Crystals from Linear-Response Theory. Physical Review Letters, 1987, 59, 2662-2665.	7.8	87
29	Isolation, Structure, and Electronic Calculations of the Heterofullerene Salt K6C59N. Science, 1996, 271, 1833-1835.	12.6	75
30	Adsorption of pairs of NOx molecules on single-walled carbon nanotubes and formation of NO+NO3 from NO2. Surface Science, 2009, 603, 3234-3238.	1.9	70
31	Low-temperature structures of C4 and C10 from the Carâ€"Parrinello method: singlet states. Chemical Physics Letters, 1990, 173, 449-455.	2.6	61
32	Amphoteric behavior ofH0in GaAs. Physical Review B, 1990, 42, 1864-1867.	3.2	56
33	Theoretical analysis of the 3-k magnetic structure and distortion of uranium dioxide. Journal of Magnetism and Magnetic Materials, 1987, 67, 75-87.	2.3	53
34	Structure and Passivation Effects of Mono- and Dihydrogen Complexes inGaAsyN1â^'yAlloys. Physical Review Letters, 2002, 89, 216401.	7.8	52
35	Theory of the metal-nonmagnetic Mott-Jahn-Teller insulator transition inA4C60. Physical Review B, 2000, 62, 7619-7624.	3.2	49
36	The ordinary and matrix continued fractions in the theoretical analysis of Hermitian and relaxation operators. Applied Numerical Mathematics, 1988, 4, 273-295.	2.1	45

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37	Isotopically resolved Raman spectra ofC60. Physical Review Letters, 1994, 72, 3359-3362.	7.8	44
38	Molecular structure and chemical bonding inK3C60andK6C60. Physical Review B, 1995, 51, 2087-2097.	3.2	44
39	Interfacial Engineering of P3HT/ZnO Hybrid Solar Cells Using Phthalocyanines: A Joint Theoretical and Experimental Investigation. Advanced Energy Materials, 2014, 4, 1301694.	19.5	42
40	Anomalous electronic behaviour of Na superfullerides: theory and experiment. Europhysics Letters, 1996, 34, 699-704.	2.0	39
41	Infrared reflectivity by transverse-optical phonons in (GaAs)m/(AlAs)nultrathin-layer superlattices. Physical Review B, 1991, 43, 14754-14757.	3.2	38
42	H passivation of Si impurities in GaAs. Physical Review B, 1991, 43, 2446-2449.	3.2	37
43	Zinc Oxideâ€“Zinc Phthalocyanine Interface for Hybrid Solar Cells. Journal of Physical Chemistry C, 2012, 116, 15439-15448.	3.1	36
44	Nitrogen passivation by atomic hydrogen inGaAsyN1â^'yandInxGa1â^'xAsyN1â^'yalloys. Physical Review B, 2003, 68, .	3.2	34
45	Microscopic structure of the substitutional Al defect in Î± quartz. Physical Review B, 2000, 61, 2621-2625.	3.2	33
46	Zn induced structural aggregation patterns of Î²-amyloid peptides by first-principle simulations and XAS measurements. Metallomics, 2012, 4, 156-165.	2.4	33
47	Reconstruction of frozen-core all-electron orbitals from pseudo-orbitals. Journal of Chemical Physics, 2001, 115, 5791-5795.	3.0	32
48	A hybrid zinc phthalocyanine/zinc oxide system for photovoltaic devices: a DFT and TDDFPT theoretical investigation. Journal of Materials Chemistry, 2012, 22, 440-446.	6.7	32
49	The low frequency vibrational modes of green fluorescent proteins. Chemical Physics, 2003, 287, 33-42.	1.9	31
50	Photocatalytic and Photovoltaic Properties of TiO₂ Nanoparticles Investigated by Ab Initio Simulations. Journal of Physical Chemistry C, 2014, 118, 29928-29942.	3.1	31
51	Effects of Doping on the Vibrational Properties ofC60from First Principles:K6C60. Physical Review Letters, 1996, 76, 4915-4918.	7.8	30
52	Fast hybrid density-functional computations using plane-wave basis sets. Electronic Structure, 2019, 1, 015009.	2.8	29
53	Effects of Strain and Local Charge on the Formation of Deep Defects in III-V Ternary Alloys. Physical Review Letters, 2000, 84, 3923-3926.	7.8	28
54	Density Functional Theory Study of the Structure and 13C Chemical Shifts of Retinylidene Iminium Salts. Journal of Physical Chemistry B, 2000, 104, 9048-9053.	2.6	28

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55	Ground state properties of cesium dimers from ab initio pseudopotential approaches. Journal of Chemical Physics, 1989, 90, 7306-7312.	3.0	27
56	Phonon softening and high-pressure low-symmetry phases of cesium iodide. Physical Review Letters, 1992, 69, 1069-1072.	7.8	27
57	Absence of metal clusters and appearance of new electron states inNa6C60. Physical Review Letters, 1994, 72, 848-851.	7.8	27
58	Ab initio Theoretical Investigation of Phthalocyanineâ^'Semiconductor Hybrid Systems. Chemistry of Materials, 2009, 21, 4555-4567.	6.7	27
59	Coordination and Haptotropic Rearrangement of Cr(CO)3on (n,0) Nanotube Sidewalls:Â A Dynamical Density Functional Study. Journal of Physical Chemistry B, 2004, 108, 5243-5249.	2.6	25
60	Vibrational frequencies of Si-P-H complexes in crystalline silicon: A theoretical study. Physical Review B, 1990, 42, 3175-3178.	3.2	23
61	High-pressure low-symmetry phases of cesium halides. Physical Review B, 1995, 51, 8060-8068.	3.2	23
62	Strain and alloying effects on the electronic and vibrational properties of InyAl1â^'yAs on InP. Journal of Applied Physics, 1995, 78, 470-477.	2.5	23
63	Density-Functional Perturbation Theory. , 2005, , 195-214.		22
64	Unit cell restricted Bloch functions basis for first-principle transport models: Theory and application. Physical Review B, 2020, 102, .	3.2	19
65	The Classical and Generalized Moment Problem in the Theory of Relaxation. Physica Status Solidi (B): Basic Research, 1985, 128, 643-652.	1.5	18
66	Raman cross section for the pentagonal-pinch mode in buckminsterfullerene C60. Chemical Physics Letters, 1997, 270, 129-134.	2.6	17
67	Comment on â€œNoncovalent functionalization of carbon nanotubes by aromatic organic moleculesâ€• [Appl. Phys. Lett. 82, 3746 (2003)]. Applied Physics Letters, 2004, 84, 3936-3937.	3.3	17
68	SixC1â^'xO2 alloys: A possible route to stabilize carbon-based silica-like solids?. Solid State Communications, 2007, 144, 273-276.	1.9	16
69	Quantitative local environment characterization in amorphous oxides. Physical Review B, 2010, 81, .	3.2	16
70	Theoretical Design of Coupled Organic-Inorganic Systems. Physical Review Letters, 2008, 101, 126805.	7.8	14
71	The interactions of nitrogen dioxide with graphene-stabilized Rh clusters: a DFT study. Physical Chemistry Chemical Physics, 2013, 15, 15896.	2.8	14
72	Structure, electronic properties, and formation mechanisms of hydrogen-nitrogen complexes inGaPyN1â^'yalloys. Physical Review B, 2004, 69, .	3.2	13

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73	Pressure-induced structural instability of cesium halides fromab initiopseudopotential techniques. Physical Review B, 1987, 35, 765-769.	3.2	12
74	First-Principles Molecular Dynamics. , 2005, , 59-76.		12
75	A Performance Study of Quantum ESPRESSOâ€™s PWscf Code on Multi-core and GPU Systems. Lecture Notes in Computer Science, 2018, , 67-87.	1.3	12
76	Structure, kinetics, and passivation of hydrogen-acceptor complexes in gallium arsenide: A theoretical study. Physical Review B, 1998, 57, 12923-12931.	3.2	10
77	Electron correlation effects on the hydrogen passivation ofMnxGa1â^'xAsdilute magnetic semiconductors. Physical Review B, 2005, 72, .	3.2	10
78	Improved understanding of metalâ€“graphene contacts. Microelectronic Engineering, 2019, 216, 111035.	2.4	10
79	Theory of electronic states in lattices and superlattices. Rivista Del Nuovo Cimento, 1990, 13, 1-80.	5.7	9
80	Vibrational Properties of DsRed Model Chromophores. ChemPhysChem, 2005, 6, 1786-1788.	2.1	9
81	First-principles calculations of hydrogen in bulk GaAs. Physica B: Condensed Matter, 1991, 170, 392-396.	2.7	8
82	A first-principles derived parametrization for the adiabatic bond charge model. Solid State Communications, 1995, 96, 49-52.	1.9	8
83	Ab initiomolecular dynamics study of amorphousCdTeOxalloys: Structural properties. Physical Review B, 2009, 79, .	3.2	8
84	3. Density-Functional Perturbation Theory for Quasi-Harmonic Calculations. , 2010, , 39-58.		8
85	Hartree-Fock energy bands in molecular crystals: Solid hydrogen in the cubic phase. Physical Review B, 1984, 30, 7187-7193.	3.2	7
86	Silicon-hydrogen-acceptor complexes in crystalline silicon. Physical Review B, 1992, 45, 11744-11748.	3.2	7
87	Carbonyl group generation on single-wall carbon nanotubes with nitric acid: A theoretical description. Chemical Physics Letters, 2013, 582, 123-128.	2.6	7
88	Investigation of structural, electronic and magnetic properties of breathing metalâ€“organic framework MIL-47(Mn): a first principles approach. RSC Advances, 2020, 10, 4786-4794.	3.6	7
89	Multiple-scattering approach to the propagation of electromagnetic waves in heterogeneous media. Physical Review B, 1986, 34, 2952-2955.	3.2	6
90	Core-level shift analysis of amorphous CdTeO x materials. Journal of Materials Science, 2010, 45, 5071-5076.	3.7	6

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91	Engineering of metal-MoS2 contacts to overcome Fermi level pinning. Solid-State Electronics, 2022, 194, 108378.	1.4	6
92	Positional disorder in ammonia borane at ambient conditions. Physical Review B, 2014, 89, .	3.2	5
93	Structure constants in the Green's-function method: A new analytic evaluation. Physical Review B, 1983, 27, 7553-7562.	3.2	4
94	Structural and vibrational properties of the Si-H-Al complex in crystalline silicon. Physical Review B, 1991, 44, 3399-3402.	3.2	4
95	Hydrogen-induced states near the GaAs band edges. Physical Review B, 1999, 59, 4869-4880.	3.2	3
96	Electron Densities and Related Properties from the ab-initio Simulation of Crystalline Solids. , 2011, , 79-132.		3
97	Large-Scale Electronic Structure Calculations in Solids. , 1995, , 67-86.		3
98	High Pressure Lattice Instabilities and Structural Phase Transformations in Solids from Ab-Initio Lattice Dynamics. Materials Research Society Symposia Proceedings, 1997, 499, 233.	0.1	2
99	DFT study of graphene doping due to metal contacts. , 2019, , .		2
100	Phonon Spectra of Ultrathin GaAs/AlAs Superlattices. NATO ASI Series Series B: Physics, 1991, , 39-52.	0.2	2
101	Structural and Electronic Properties of C60 and C60 Derivatives in the Solid Phases: Calculations Based on Density-Functional Theory. Physics and Chemistry of Materials With Low-dimensional Structures, 2000, , 291-329.	1.0	2
102	Ab Initio Calculation of Phonon Spectra in Semiconductors: from Pure Crystals to Alloys and Superlattices. , 1993, , 243-277.		1
103	Defect engineering in IIIâ€“V ternary alloys: effects of strain and local charge on the formation of substitutional and interstitial native defects. Physica B: Condensed Matter, 2001, 308-310, 846-849.	2.7	1
104	Frontispiece: Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, .	3.3	1
105	Measuring Shared Electrons in Extended Molecular Systems: Covalent Bonds from Plane-Wave Representation of Wave Function. Molecules, 2021, 26, 4044.	3.8	1
106	Density-Functional Perturbation Theory. , 2005, , 195-214.		1
107	Structure and Thermodynamics of SiGe Alloys from Computational Alchemy. , 1992, , 133-149.		1
108	First-Principles Molecular Dynamics. , 2005, , 59-76.		1

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109	First-principles calculations of hydrogen in bulk GaAs. , 1991, , 392-396.		0
110	Equilibrium Sites and Relative Stability of Atomic and Molecular Hydrogen in GaAs. Materials Science Forum, 1992, 83-87, 611-616.	0.3	0
111	Vibrational properties of isolated AlAs monolayers embedded in GaAs: a theoretical study of the effects of disorder. Applied Surface Science, 1992, 56-58, 617-621.	6.1	0
112	Defect engineering in IIIâ€“V ternary alloys: Effects of strain and local charge on the formation of native deep defects. Nuclear Instruments & Methods in Physics Research B, 2002, 186, 229-233.	1.4	0
113	Condensation Energy and Tc within the Density Functional Theory for Superconductors. AIP Conference Proceedings, 2005, , .	0.4	0