# Paolo Giannozzi

## List of Publications by Year in descending order

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|---|---|---|---|
| 113 papers | 40,766 citations | 93792 39 h-index | 39744 98 g-index |
| 114 all docs | 114 docs citations | 114 times ranked | 34956 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Engineering of metal-MoS2 contacts to overcome Fermi level pinning. Solid-State Electronics, 2022, 194, 108378. | 0.8 | 6 |
| 2 | Measuring Shared Electrons in Extended Molecular Systems: Covalent Bonds from Plane-Wave Representation of Wave Function. Molecules, 2021, 26, 4044. | 1.7 | 1 |
| 3 | Unit cell restricted Bloch functions basis for first-principle transport models: Theory and application. Physical Review B, 2020, 102, . | 1.1 | 19 |
| 4 | Q<scp>uantum</scp> ESPRESSO toward the exascale. Journal of Chemical Physics, 2020, 152, 154105. | 1.2 | 796 |
| 5 | 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. | 1.7 | 7 |
| 6 | DFT study of graphene doping due to metal contacts. , 2019, , . | | 2 |
| 7 | Fast hybrid density-functional computations using plane-wave basis sets. Electronic Structure, 2019, 1, 015009. | 1.0 | 29 |
| 8 | Improved understanding of metalâ€“graphene contacts. Microelectronic Engineering, 2019, 216, 111035. | 1.1 | 10 |
| 9 | Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905. | 1.7 | 108 |
| 10 | Frontispiece: Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, . | 1.7 | 1 |
| 11 | A Performance Study of Quantum ESPRESSOâ€™s PWscf Code on Multi-core and GPU Systems. Lecture Notes in Computer Science, 2018, , 67-87. | 1.0 | 12 |
| 12 | Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901. | 0.7 | 4,303 |
| 13 | Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000. | 6.0 | 1,113 |
| 14 | Photocatalytic and Photovoltaic Properties of TiO<sub>2</sub> Nanoparticles Investigated by Ab Initio Simulations. Journal of Physical Chemistry C, 2014, 118, 29928-29942. | 1.5 | 31 |
| 15 | Positional disorder in ammonia borane at ambient conditions. Physical Review B, 2014, 89, . | 1.1 | 5 |
| 16 | Interfacial Engineering of P3HT/ZnO Hybrid Solar Cells Using Phthalocyanines: A Joint Theoretical and Experimental Investigation. Advanced Energy Materials, 2014, 4, 1301694. | 10.2 | 42 |
| 17 | The interactions of nitrogen dioxide with graphene-stabilized Rh clusters: a DFT study. Physical Chemistry Chemical Physics, 2013, 15, 15896. | 1.3 | 14 |
| 18 | Carbonyl group generation on single-wall carbon nanotubes with nitric acid: A theoretical description. Chemical Physics Letters, 2013, 582, 123-128. | 1.2 | 7 |

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| 19 | Reaction Pathways for Oxygen Evolution Promoted by Cobalt Catalyst. Journal of the American Chemical Society, 2013, 135, 15353-15363. | 6.6 | 228 |
| 20 | Zn induced structural aggregation patterns of Î²-amyloid peptides by first-principle simulations and XAS measurements. Metallomics, 2012, 4, 156-165. | 1.0 | 33 |
| 21 | 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 |
| 22 | Zinc Oxideâ€“Zinc Phthalocyanine Interface for Hybrid Solar Cells. Journal of Physical Chemistry C, 2012, 116, 15439-15448. | 1.5 | 36 |
| 23 | Electron Densities and Related Properties from the ab-initio Simulation of Crystalline Solids. , 2011, , 79-132. | | 3 |
| 24 | Density-Functional Perturbation Theory for Quasi-Harmonic Calculations. Reviews in Mineralogy and Geochemistry, 2010, 71, 39-57. | 2.2 | 265 |
| 25 | Core-level shift analysis of amorphous CdTeO x materials. Journal of Materials Science, 2010, 45, 5071-5076. | 1.7 | 6 |
| 26 | 3. Density-Functional Perturbation Theory for Quasi-Harmonic Calculations. , 2010, , 39-58. | | 8 |
| 27 | Quantitative local environment characterization in amorphous oxides. Physical Review B, 2010, 81, . | 1.1 | 16 |
| 28 | Ab initiomolecular dynamics study of amorphousCdTeOxalloys: Structural properties. Physical Review B, 2009, 79, . | 1.1 | 8 |
| 29 | Adsorption of pairs of NOx molecules on single-walled carbon nanotubes and formation of NO+NO3 from NO2. Surface Science, 2009, 603, 3234-3238. | 0.8 | 70 |
| 30 | QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502. | 0.7 | 18,183 |
| 31 | Ab initio Theoretical Investigation of Phthalocyanineâ^'Semiconductor Hybrid Systems. Chemistry of Materials, 2009, 21, 4555-4567. | 3.2 | 27 |
| 32 | Gas adsorption on graphene doped with B, N, Al, and S: A theoretical study. Applied Physics Letters, 2009, 95, . | 1.5 | 643 |
| 33 | Theoretical Design of Coupled Organic-Inorganic Systems. Physical Review Letters, 2008, 101, 126805. | 2.9 | 14 |
| 34 | SixC1â^'xO2 alloys: A possible route to stabilize carbon-based silica-like solids?. Solid State Communications, 2007, 144, 273-276. | 0.9 | 16 |
| 35 | Vibrational Properties of DsRed Model Chromophores. ChemPhysChem, 2005, 6, 1786-1788. | 1.0 | 9 |
| 36 | Condensation Energy and Tc within the Density Functional Theory for Superconductors. AIP Conference Proceedings, 2005, , . | 0.3 | 0 |

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| 37 | Electron correlation effects on the hydrogen passivation ofMnxGa1â^'xAsdilute magnetic semiconductors. Physical Review B, 2005, 72, . | 1.1 | 10 |
| 38 | Density-Functional Perturbation Theory. , 2005, , 195-214. | | 22 |
| 39 | First-principles codes for computational crystallography in the Quantum-ESPRESSO package. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, . | 0.4 | 177 |
| 40 | First-Principles Molecular Dynamics. , 2005, , 59-76. | | 12 |
| 41 | Density-Functional Perturbation Theory. , 2005, , 195-214. | | 1 |
| 42 | First-Principles Molecular Dynamics. , 2005, , 59-76. | | 1 |
| 43 | Structure, electronic properties, and formation mechanisms of hydrogen-nitrogen complexes inGaPyN1â^'yalloys. Physical Review B, 2004, 69, . | 1.1 | 13 |
| 44 | 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. | 1.2 | 148 |
| 45 | 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. | 1.5 | 17 |
| 46 | 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. | 1.2 | 25 |
| 47 | First-principle molecular dynamics with ultrasoft pseudopotentials: Parallel implementation and application to extended bioinorganic systems. Journal of Chemical Physics, 2004, 120, 5903-5915. | 1.2 | 95 |
| 48 | The low frequency vibrational modes of green fluorescent proteins. Chemical Physics, 2003, 287, 33-42. | 0.9 | 31 |
| 49 | Oxygen adsorption on graphite and nanotubes. Journal of Chemical Physics, 2003, 118, 1003-1006. | 1.2 | 261 |
| 50 | Nitrogen passivation by atomic hydrogen inGaAsyN1â^'yandInxGa1â^'xAsyN1â^'yalloys. Physical Review B, 2003, 68, . | 1.1 | 34 |
| 51 | Structure and Passivation Effects of Mono- and Dihydrogen Complexes inGaAsyN1â^'yAlloys. Physical Review Letters, 2002, 89, 216401. | 2.9 | 52 |
| 52 | 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. | 0.6 | 0 |
| 53 | Phonons and related crystal properties from density-functional perturbation theory. Reviews of Modern Physics, 2001, 73, 515-562. | 16.4 | 7,534 |
| 54 | 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. | 1.2 | 230 |

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| 55 | 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. | 1.3 | 1 |
| 56 | Reconstruction of frozen-core all-electron orbitals from pseudo-orbitals. Journal of Chemical Physics, 2001, 115, 5791-5795. | 1.2 | 32 |
| 57 | Microscopic structure of the substitutional Al defect in Î± quartz. Physical Review B, 2000, 61, 2621-2625. | 1.1 | 33 |
| 58 | Theory of the metal-nonmagnetic Mott-Jahn-Teller insulator transition inA4C60. Physical Review B, 2000, 62, 7619-7624. | 1.1 | 49 |
| 59 | Effects of Strain and Local Charge on the Formation of Deep Defects in III-V Ternary Alloys. Physical Review Letters, 2000, 84, 3923-3926. | 2.9 | 28 |
| 60 | Density Functional Theory Study of the Structure and 13C Chemical Shifts of Retinylidene Iminium Salts. Journal of Physical Chemistry B, 2000, 104, 9048-9053. | 1.2 | 28 |
| 61 | 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 |
| 62 | Hydrogen-induced states near the GaAs band edges. Physical Review B, 1999, 59, 4869-4880. | 1.1 | 3 |
| 63 | Structure, kinetics, and passivation of hydrogen-acceptor complexes in gallium arsenide: A theoretical study. Physical Review B, 1998, 57, 12923-12931. | 1.1 | 10 |
| 64 | 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 |
| 65 | Raman cross section for the pentagonal-pinch mode in buckminsterfullerene C60. Chemical Physics Letters, 1997, 270, 129-134. | 1.2 | 17 |
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| 67 | Effects of Doping on the Vibrational Properties ofC60from First Principles:K6C60. Physical Review Letters, 1996, 76, 4915-4918. | 2.9 | 30 |
| 68 | Anomalous electronic behaviour of Na superfullerides: theory and experiment. Europhysics Letters, 1996, 34, 699-704. | 0.7 | 39 |
| 69 | Structure and bonding in cisplatin and other Pt(II) complexes. Chemical Physics Letters, 1995, 234, 50-56. | 1.2 | 91 |
| 70 | A first-principles derived parametrization for the adiabatic bond charge model. Solid State Communications, 1995, 96, 49-52. | 0.9 | 8 |
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| 72 | High-pressure low-symmetry phases of cesium halides. Physical Review B, 1995, 51, 8060-8068. | 1.1 | 23 |

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| 73 | Strain and alloying effects on the electronic and vibrational properties of InyAl1â^'yAs on InP. Journal of Applied Physics, 1995, 78, 470-477. | 1.1 | 23 |
| 74 | Large-Scale Electronic Structure Calculations in Solids. , 1995, , 67-86. | | 3 |
| 75 | Absence of metal clusters and appearance of new electron states inNa6C60. Physical Review Letters, 1994, 72, 848-851. | 2.9 | 27 |
| 76 | Isotopically resolved Raman spectra ofC60. Physical Review Letters, 1994, 72, 3359-3362. | 2.9 | 44 |
| 77 | Vibrational and dielectric properties of C60 from densityâ€functional perturbation theory. Journal of Chemical Physics, 1994, 100, 8537-8539. | 1.2 | 184 |
| 78 | Ab initiolattice dynamics of diamond. Physical Review B, 1993, 48, 3156-3163. | 1.1 | 298 |
| 79 | Ab Initio Calculation of Phonon Spectra in Semiconductors: from Pure Crystals to Alloys and Superlattices. , 1993, , 243-277. | | 1 |
| 80 | Second-order Raman spectra of diamond fromab initiophonon calculations. Physical Review B, 1993, 48, 3164-3170. | 1.1 | 94 |
| 81 | Equilibrium Sites and Relative Stability of Atomic and Molecular Hydrogen in GaAs. Materials Science Forum, 1992, 83-87, 611-616. | 0.3 | 0 |
| 82 | Silicon-hydrogen-acceptor complexes in crystalline silicon. Physical Review B, 1992, 45, 11744-11748. | 1.1 | 7 |
| 83 | Phonon softening and high-pressure low-symmetry phases of cesium iodide. Physical Review Letters, 1992, 69, 1069-1072. | 2.9 | 27 |
| 84 | Effects of disorder on the Raman spectra of GaAs/AlAs superlattices. Physical Review B, 1992, 45, 4280-4288. | 1.1 | 88 |
| 85 | Atomic and molecular hydrogen in gallium arsenide: A theoretical study. Physical Review B, 1992, 46, 4621-4629. | 1.1 | 89 |
| 86 | Towards Very Large-Scale Electronic-Structure Calculations. Europhysics Letters, 1992, 17, 547-552. | 0.7 | 155 |
| 87 | Thirteenâ€atom clusters: Equilibrium geometries, structural transformations, and trends in Na, Mg, Al, and Si. Journal of Chemical Physics, 1992, 96, 1248-1256. | 1.2 | 140 |
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| 90 | Ab initiocalculation of phonon dispersions in semiconductors. Physical Review B, 1991, 43, 7231-7242. | 1.1 | 1,619 |

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| 93 | H passivation of Si impurities in GaAs. Physical Review B, 1991, 43, 2446-2449. | 1.1 | 37 |
| 94 | Infrared reflectivity by transverse-optical phonons in (GaAs)m/(AlAs)nultrathin-layer superlattices. Physical Review B, 1991, 43, 14754-14757. | 1.1 | 38 |
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| 96 | Structure and thermodynamics ofSixGe1â^'xalloys fromab initioMonte Carlo simulations. Physical Review Letters, 1991, 66, 2116-2119. | 2.9 | 155 |
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| 101 | Phonon dispersions inGaxAl1â^'xAs alloys. Physical Review Letters, 1990, 65, 84-87. | 2.9 | 108 |
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| 110 | Multiple-scattering approach to the propagation of electromagnetic waves in heterogeneous media. Physical Review B, 1986, 34, 2952-2955. | 1.1 | 6 |
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| 112 | Hartree-Fock energy bands in molecular crystals: Solid hydrogen in the cubic phase. Physical Review B, 1984, 30, 7187-7193. | 1.1 | 7 |
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