Luigi Genovese

List of Publications by Year
in descending order

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77 papers	6,791 citations	201575 27 h-index	74108 75 g-index
86 all docs	86 docs citations	86 times ranked	8224 citing authors

#	Article	IF	Citations
1	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	3.0	2,297
2	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
3	Recent developments in the ABINIT software package. Computer Physics Communications, 2016, 205, 106-131.	3.0	662
4	Daubechies wavelets as a basis set for density functional pseudopotential calculations. Journal of Chemical Physics, 2008, 129, 014109.	1.2	289
5	Efficient solution of Poissonâ€™s equation with free boundary conditions. Journal of Chemical Physics, 2006, 125, 074105.	1.2	176
6	Energy Landscape of Fullerene Materials: A Comparison of Boron to Boron Nitride and Carbon. Physical Review Letters, 2011, 106, 225502.	2.9	169
7	Accurate and efficient linear scaling DFT calculations with universal applicability. Physical Chemistry Chemical Physics, 2015, 17, 31360-31370.	1.3	158
8	Daubechies wavelets for linear scaling density functional theory. Journal of Chemical Physics, 2014, 140, 204110.	1.2	140
9	Efficient and accurate three-dimensional Poisson solver for surface problems. Journal of Chemical Physics, 2007, 127, 054704.	1.2	102
10	Challenges in large scale quantum mechanical calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1290.	6.2	98
11	Norm-conserving pseudopotentials with chemical accuracy compared to all-electron calculations. Journal of Chemical Physics, 2013, 138, 104109.	1.2	95
12	A generalized Poisson and Poisson-Boltzmann solver for electrostatic environments. Journal of Chemical Physics, 2016, 144, 014103.	1.2	88
13	Density functional theory calculation on many-cores hybrid central processing unit-graphic processing unit architectures. Journal of Chemical Physics, 2009, 131, 034103.	1.2	87
14	Optimized energy landscape exploration using the ab initio based activation-relaxation technique. Journal of Chemical Physics, 2011, 135, 034102.	1.2	81
15	Soft-Sphere Continuum Solvation in Electronic-Structure Calculations. Journal of Chemical Theory and Computation, 2017, 13, 3829-3845.	2.3	76
16	Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194110.	1.2	60
17	X-Ray Magnetic Circular Dichroism Measurements in Ni up to 200ÂGPa: Resistant Ferromagnetism. Physical Review Letters, 2011, 107, 237202.	2.9	56
18	Discovery of SARS-CoV-2 M^{pro} peptide inhibitors from modelling substrate and ligand binding. Chemical Science, 2021, 12, 13686-13703.	3.7	54

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19	Daubechies wavelets for high performance electronic structure calculations: The BigDFT project. Comptes Rendus - Mecanique, 2011, 339, 149-164.	2.1	53
20	Structural metastability of endohedral silicon fullerenes. Physical Review B, 2010, 81, .	1.1	39
21	Toward Fast and Accurate Evaluation of Charge On-Site Energies and Transfer Integrals in Supramolecular Architectures Using Linear Constrained Density Functional Theory (CDFT)-Based Methods. Journal of Chemical Theory and Computation, 2015, 11, 2077-2086.	2.3	38
22	First-principles prediction of stable SiC cage structures and their synthesis pathways. Physical Review B, 2010, 82, .	1.1	37
23	Low-energy boron fullerenes: Role of disorder and potential synthesis pathways. Physical Review B, 2011, 83, .	1.1	37
24	Efficient and accurate solver of the three-dimensional screened and unscreened Poisson's equation with generic boundary conditions. Journal of Chemical Physics, 2012, 137, 134108.	1.2	36
25	Revisiting the domain model for lithium intercalated graphite. Applied Physics Letters, 2013, 103, .	1.5	33
26	Energy landscape of silicon systems and its description by force fields, tight binding schemes, density functional methods, and quantum Monte Carlo methods. Physical Review B, 2010, 81, .	1.1	31
27	Selecting boron fullerenes by cage-doping mechanisms. Journal of Chemical Physics, 2013, 138, 184302.	1.2	29
28	Quantum-transport simulations with the Wigner-function formalism: Failure of conventional boundary-condition schemes. Europhysics Letters, 2006, 74, 1060-1066.	0.7	27
29	Stable structures of exohedrally decorated C60-fullerenes. Carbon, 2018, 129, 847-853.	5.4	27
30	Tunable magnetic states in hexagonal boron nitride sheets. Applied Physics Letters, 2012, 101, .	1.5	26
31	Linear scaling DFT calculations for large tungsten systems using an optimized local basis. Nuclear Materials and Energy, 2018, 15, 64-70.	0.6	26
32	The effect of ionization on the global minima of small and medium sized silicon and magnesium clusters. Journal of Chemical Physics, 2011, 134, 124302.	1.2	25
33	Wet Environment Effects for Ethanol and Water Adsorption on Anatase TiO₂ (101) Surfaces. Journal of Physical Chemistry C, 2020, 124, 2406-2419.	1.5	24
34	Metallofullerenes as fuel cell electrocatalysts: A theoretical investigation of adsorbates on C59Pt. Physical Chemistry Chemical Physics, 2010, 12, 9406.	1.3	23
35	Efficient Computation of Sparse Matrix Functions for Large-Scale Electronic Structure Calculations: The <scp>CheSS</scp> Library. Journal of Chemical Theory and Computation, 2017, 13, 4684-4698.	2.3	23
36	Static Polarizabilities at the Basis Set Limit: A Benchmark of 124 Species. Journal of Chemical Theory and Computation, 2020, 16, 4874-4882.	2.3	23

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37	Noncollinear magnetic ordering in compressed FePd<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn mathvariant="bold">3</mml:mn></mml:msub></mml:math>ordered alloy: A first principles study. Physical Review B, 2012, 86, .	1.1	19
38	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	1.2	19
39	Complexity Reduction in Density Functional Theory Calculations of Large Systems: System Partitioning and Fragment Embedding. Journal of Chemical Theory and Computation, 2020, 16, 2952-2964.	2.3	19
40	A wavelet-based Projector Augmented-WaveÂ(PAW) method: Reaching frozen-core all-electron precision with a systematic, adaptive and localized wavelet basis set. Computer Physics Communications, 2016, 208, 1-8.	3.0	18
41	Complexity Reduction in Large Quantum Systems: Fragment Identification and Population Analysis via a Local Optimized Minimal Basis. Journal of Chemical Theory and Computation, 2017, 13, 4079-4088.	2.3	18
42	Wavelet-based linear-response time-dependent density-functional theory. Chemical Physics, 2012, 402, 29-40.	0.9	16
43	Fragment approach to constrained density functional theory calculations using Daubechies wavelets. Journal of Chemical Physics, 2015, 142, 234105.	1.2	16
44	Affordable and accurate large-scale hybrid-functional calculations on GPU-accelerated supercomputers. Journal of Physics Condensed Matter, 2018, 30, 095901.	0.7	16
45	Designing a bioremediator: mechanistic models guide cellular and molecular specialization. Current Opinion in Biotechnology, 2020, 62, 98-105.	3.3	16
46	Density functional theory calculations of large systems: Interplay between fragments, observables, and computational complexity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1574.	6.2	16
47	Metastable exohedrally decorated Borospherene B40. Scientific Reports, 2017, 7, 7618.	1.6	15
48	Surface reconstruction of fluorites in vacuum and aqueous environment. Physical Review Materials, 2017, 1, .	0.9	15
49	Phonon-limited carrier mobility and resistivity from carbon nanotubes to graphene. Physical Review B, 2015, 92, .	1.1	14
50	The phase diagram of the three-dimensionalZ2 gauge Higgs system at zero and finite temperature. Nuclear Physics, Section B, Proceedings Supplements, 2003, 119, 894-899.	0.5	11
51	Adsorption of small NaCl clusters on surfaces of silicon nanostructures. Nanotechnology, 2009, 20, 445301.	1.3	11
52	Use of the Dual Potential to Rationalize the Occurrence of Some DNA Lesions (Pyrimidic Dimers). Journal of Physical Chemistry A, 2011, 115, 8032-8040.	1.1	11
53	A customized 3D GPU Poisson solver for free boundary conditions. Computer Physics Communications, 2013, 184, 1815-1820.	3.0	11
54	A highly selective non-radical diazo coupling provides low cost semi-conducting carbon nanotubes. Carbon, 2014, 66, 246-258.	5.4	11

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55	Boron aggregation in the ground states of boron-carbon fullerenes. Physical Review B, 2014, 89, .	1.1	11
56	Electrochemical deposition of Ag 2 Se nanostructures. Materials Research Bulletin, 2017, 86, 10-18.	2.7	11
57	A wide class of four point functions of BPS operators in SYM at order. Nuclear Physics B, 2006, 732, 64-88.	0.9	10
58	Direct observation of single organic molecules grafted on the surface of a silicon nanowire. Scientific Reports, 2019, 9, 5647.	1.6	10
59	Common workflows for computing material properties using different quantum engines. Npj Computational Materials, 2021, 7, .	3.5	10
60	Accurate complex scaling of three dimensional numerical potentials. Journal of Chemical Physics, 2013, 138, 204111.	1.2	9
61	Multipole-preserving quadratures for the discretization of functions in real-space electronic structure calculations. Physical Chemistry Chemical Physics, 2015, 17, 31582-31591.	1.3	9
62	Towards simulation at picometer-scale resolution: Revisiting inversion domain boundaries in GaN. Physical Review B, 2018, 98, .	1.1	9
63	BOAST. International Journal of High Performance Computing Applications, 2018, 32, 28-44.	2.4	8
64	Pressure-induced structural and magnetic phase transitions in ordered and disordered equiatomic FeCo. Physical Review B, 2013, 88, .	1.1	7
65	Pseudo-fragment approach for extended systems derived from linear-scaling DFT. Journal of Physics Condensed Matter, 2019, 31, 285901.	0.7	6
66	Wavelets for electronic structure calculations. Ã‰cole ThÃ©matique De La SociÃ©tÃ© FranÃ§aise De La Neutronique, 2011, 12, 33-76.	0.2	5
67	Transport in quantum devices: modelling contacts in the Wigner formalism. Physica Status Solidi C: Current Topics in Solid State Physics, 2006, 3, 2419-2422.	0.8	3
68	Energetic and vibrational analysis of hydrogenated silicon<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>m</mml:mi></mml:math>vacancies above saturation. Physical Review B, 2014, 90, .	1.1	3
69	Rationality of the anomalous dimensions in SYM theory. Nuclear Physics B, 2005, 721, 212-228.	0.9	2
70	Overlapping Computations with Communications and I/O Explicitly Using OpenMP Based Heterogeneous Threading Models. Lecture Notes in Computer Science, 2012, , 267-270.	1.0	2
71	Influence of an external electric field on the potential-energy surface of alkali-metal-decorated C60. Physical Review A, 2018, 97, .	1.0	2
72	Locality and computational reliability of linear response calculations for molecular systems. Physical Review Materials, 2019, 3, .	0.9	2

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73	Exploring metastable states in UO₂ using hybrid functionals and dynamical mean field theory. Journal of Physics Condensed Matter, 2022, 34, 094003.	0.7	2
74	Transition-Based Constrained DFT for the Robust and Reliable Treatment of Excitations in Supramolecular Systems. Journal of Chemical Theory and Computation, 2022, 18, 3027-3038.	2.3	2
75	Quantum Non-Locality in Systems with Open Boundaries: Limitations of the Wigner function formalism. AIP Conference Proceedings, 2007, , .	0.3	0
76	Wavelet-Based Density Functional Theory Calculation on Massively Parallel Hybrid Architectures. , 2011, , 133-151.		0
77	Enhancing the Flexibility of First Principles Simulations of Materials via Wavelets. Springer Series in Materials Science, 2020, , 57-78.	0.4	0