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	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
2	Exploring metastable states in UO₂ using hybrid functionals and dynamical mean field theory. Journal of Physics Condensed Matter, 2022, 34, 094003.	0.7	2
3	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
4	Common workflows for computing material properties using different quantum engines. Npj Computational Materials, 2021, 7, .	3.5	10
5	Discovery of SARS-CoV-2 M^{pro} peptide inhibitors from modelling substrate and ligand binding. Chemical Science, 2021, 12, 13686-13703.	3.7	54
6	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
7	Designing a bioremediator: mechanistic models guide cellular and molecular specialization. Current Opinion in Biotechnology, 2020, 62, 98-105.	3.3	16
8	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	1.2	19
9	Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194110.	1.2	60
10	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
11	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
12	Enhancing the Flexibility of First Principles Simulations of Materials via Wavelets. Springer Series in Materials Science, 2020, , 57-78.	0.4	0
13	Direct observation of single organic molecules grafted on the surface of a silicon nanowire. Scientific Reports, 2019, 9, 5647.	1.6	10
14	Pseudo-fragment approach for extended systems derived from linear-scaling DFT. Journal of Physics Condensed Matter, 2019, 31, 285901.	0.7	6
15	Locality and computational reliability of linear response calculations for molecular systems. Physical Review Materials, 2019, 3, .	0.9	2
16	Affordable and accurate large-scale hybrid-functional calculations on GPU-accelerated supercomputers. Journal of Physics Condensed Matter, 2018, 30, 095901.	0.7	16
17	Linear scaling DFT calculations for large tungsten systems using an optimized local basis. Nuclear Materials and Energy, 2018, 15, 64-70.	0.6	26
18	Stable structures of exohedrally decorated C60-fullerenes. Carbon, 2018, 129, 847-853.	5.4	27

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19	BOAST. International Journal of High Performance Computing Applications, 2018, 32, 28-44.	2.4	8
20	Towards simulation at picometer-scale resolution: Revisiting inversion domain boundaries in GaN. Physical Review B, 2018, 98, .	1.1	9
21	Influence of an external electric field on the potential-energy surface of alkali-metal-decorated C60. Physical Review A, 2018, 97, .	1.0	2
22	Soft-Sphere Continuum Solvation in Electronic-Structure Calculations. Journal of Chemical Theory and Computation, 2017, 13, 3829-3845.	2.3	76
23	Metastable exohedrally decorated Borospherene B40. Scientific Reports, 2017, 7, 7618.	1.6	15
24	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
25	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
26	Challenges in large scale quantum mechanical calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1290.	6.2	98
27	Electrochemical deposition of Ag 2 Se nanostructures. Materials Research Bulletin, 2017, 86, 10-18.	2.7	11
28	Surface reconstruction of fluorites in vacuum and aqueous environment. Physical Review Materials, 2017, 1, .	0.9	15
29	A generalized Poisson and Poisson-Boltzmann solver for electrostatic environments. Journal of Chemical Physics, 2016, 144, 014103.	1.2	88
30	Recent developments in the ABINIT software package. Computer Physics Communications, 2016, 205, 106-131.	3.0	662
31	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
32	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
33	Phonon-limited carrier mobility and resistivity from carbon nanotubes to graphene. Physical Review B, 2015, 92, .	1.1	14
34	Fragment approach to constrained density functional theory calculations using Daubechies wavelets. Journal of Chemical Physics, 2015, 142, 234105.	1.2	16
35	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
36	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

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37	Accurate and efficient linear scaling DFT calculations with universal applicability. Physical Chemistry Chemical Physics, 2015, 17, 31360-31370.	1.3	158
38	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
39	A highly selective non-radical diazo coupling provides low cost semi-conducting carbon nanotubes. Carbon, 2014, 66, 246-258.	5.4	11
40	Daubechies wavelets for linear scaling density functional theory. Journal of Chemical Physics, 2014, 140, 204110.	1.2	140
41	Boron aggregation in the ground states of boron-carbon fullerenes. Physical Review B, 2014, 89, .	1.1	11
42	Accurate complex scaling of three dimensional numerical potentials. Journal of Chemical Physics, 2013, 138, 204111.	1.2	9
43	Selecting boron fullerenes by cage-doping mechanisms. Journal of Chemical Physics, 2013, 138, 184302.	1.2	29
44	Norm-conserving pseudopotentials with chemical accuracy compared to all-electron calculations. Journal of Chemical Physics, 2013, 138, 104109.	1.2	95
45	A customized 3D GPU Poisson solver for free boundary conditions. Computer Physics Communications, 2013, 184, 1815-1820.	3.0	11
46	Pressure-induced structural and magnetic phase transitions in ordered and disordered equiatomic FeCo. Physical Review B, 2013, 88, .	1.1	7
47	Revisiting the domain model for lithium intercalated graphite. Applied Physics Letters, 2013, 103, .	1.5	33
48	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
49	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
50	Tunable magnetic states in hexagonal boron nitride sheets. Applied Physics Letters, 2012, 101, .	1.5	26
51	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
52	Wavelet-based linear-response time-dependent density-functional theory. Chemical Physics, 2012, 402, 29-40.	0.9	16
53	Low-energy boron fullerenes: Role of disorder and potential synthesis pathways. Physical Review B, 2011, 83, .	1.1	37
54	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

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55	X-Ray Magnetic Circular Dichroism Measurements in Ni up to 200ÂGPa: Resistant Ferromagnetism. Physical Review Letters, 2011, 107, 237202.	2.9	56
56	Daubechies wavelets for high performance electronic structure calculations: The BigDFT project. Comptes Rendus - Mecanique, 2011, 339, 149-164.	2.1	53
57	Energy Landscape of Fullerene Materials: A Comparison of Boron to Boron Nitride and Carbon. Physical Review Letters, 2011, 106, 225502.	2.9	169
58	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
59	Optimized energy landscape exploration using the ab initio based activation-relaxation technique. Journal of Chemical Physics, 2011, 135, 034102.	1.2	81
60	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
61	Wavelet-Based Density Functional Theory Calculation on Massively Parallel Hybrid Architectures. , 2011, , 133-151.		0
62	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
63	First-principles prediction of stable SiC cage structures and their synthesis pathways. Physical Review B, 2010, 82, .	1.1	37
64	Structural metastability of endohedral silicon fullerenes. Physical Review B, 2010, 81, .	1.1	39
65	Metallofullerenes as fuel cell electrocatalysts: A theoretical investigation of adsorbates on C59Pt. Physical Chemistry Chemical Physics, 2010, 12, 9406.	1.3	23
66	Adsorption of small NaCl clusters on surfaces of silicon nanostructures. Nanotechnology, 2009, 20, 445301.	1.3	11
67	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	3.0	2,297
68	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
69	Daubechies wavelets as a basis set for density functional pseudopotential calculations. Journal of Chemical Physics, 2008, 129, 014109.	1.2	289
70	Efficient and accurate three-dimensional Poisson solver for surface problems. Journal of Chemical Physics, 2007, 127, 054704.	1.2	102
71	Quantum Non-Locality in Systems with Open Boundaries: Limitations of the Wigner function formalism. AIP Conference Proceedings, 2007, , .	0.3	0
72	A wide class of four point functions of BPS operators in SYM at order. Nuclear Physics B, 2006, 732, 64-88.	0.9	10

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73	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
74	Efficient solution of Poissonâ€™s equation with free boundary conditions. Journal of Chemical Physics, 2006, 125, 074105.	1.2	176
75	Quantum-transport simulations with the Wigner-function formalism: Failure of conventional boundary-condition schemes. Europhysics Letters, 2006, 74, 1060-1066.	0.7	27
76	Rationality of the anomalous dimensions in SYM theory. Nuclear Physics B, 2005, 721, 212-228.	0.9	2
77	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