Luca M Ghiringhelli

List of Publications by Year
in descending order

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67 papers	4,728 citations	147801 31 h-index	102487 66 g-index
73 all docs	73 docs citations	73 times ranked	5544 citing authors

#	Article	IF	Citations
1	New tolerance factor to predict the stability of perovskite oxides and halides. Science Advances, 2019, 5, eaav0693.	10.3	778
2	Big Data of Materials Science: Critical Role of the Descriptor. Physical Review Letters, 2015, 114, 105503.	7.8	658
3	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	1.1	445
4	SISSO: A compressed-sensing method for identifying the best low-dimensional descriptor in an immensity of offered candidates. Physical Review Materials, 2018, 2, .	2.4	349
5	Insightful classification of crystal structures using deep learning. Nature Communications, 2018, 9, 2775.	12.8	237
6	Improved long-range reactive bond-order potential for carbon. I. Construction. Physical Review B, 2005, 72, .	3.2	230
7	Modeling the Phase Diagram of Carbon. Physical Review Letters, 2005, 94, 145701.	7.8	119
8	Learning physical descriptors for materials science by compressed sensing. New Journal of Physics, 2017, 19, 023017.	2.9	100
9	Simultaneous learning of several materials properties from incomplete databases with multi-task SISSO. JPhys Materials, 2019, 2, 024002.	4.2	97
10	GAtor: A First-Principles Genetic Algorithm for Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2018, 14, 2246-2264.	5.3	86
11	Surface-induced crystallization in supercooled tetrahedral liquids. Nature Materials, 2009, 8, 726-730.	27.5	84
12	Theory and hierarchical calculations of the structure and energetics of [0001] tilt grain boundaries in graphene. Physical Review B, 2011, 84, .	3.2	84
13	Towards efficient data exchange and sharing for big-data driven materials science: metadata and data formats. Npj Computational Materials, 2017, 3, .	8.7	79
14	Uncovering structure-property relationships of materials by subgroup discovery. New Journal of Physics, 2017, 19, 013031.	2.9	77
15	Stability and Metastability of Clusters in a Reactive Atmosphere: Theoretical Evidence for Unexpected Stoichiometries of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Mg</mml:mi><mml:mi>M</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:math>. Physical Review Letters, 2013, 111, 135501.	7.8	72
16	Competing Adsorption between Hydrated Peptides and Water onto Metal Surfaces: From Electronic to Conformational Properties. Journal of the American Chemical Society, 2008, 130, 13460-13464.	13.7	68
17	Identifying domains of applicability of machine learning models for materials science. Nature Communications, 2020, 11, 4428.	12.8	66
18	State-of-the-art models for the phase diagram of carbon and diamond nucleation. Molecular Physics, 2008, 106, 2011-2038.	1.7	58

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19	Not so loosely bound rare gas atoms: finite-temperature vibrational fingerprints of neutral gold-cluster complexes. New Journal of Physics, 2013, 15, 083003.	2.9	56
20	Autocatalytic and Cooperatively Stabilized Dissociation of Water on a Stepped Platinum Surface. Journal of the American Chemical Society, 2012, 134, 19217-19222.	13.7	53
21	Interaction of Hydrated Amino Acids with Metal Surfaces:â€‰ A Multiscale Modeling Description. Journal of Physical Chemistry C, 2007, 111, 2631-2642.	3.1	50
22	Improved long-range reactive bond-order potential for carbon. II. Molecular simulation of liquid carbon. Physical Review B, 2005, 72, .	3.2	48
23	Phenylalanine near Inorganic Surfaces:Â Conformational Statistics vs Specific Chemistry. Journal of the American Chemical Society, 2008, 130, 2634-2638.	13.7	46
24	Artificial-intelligence-driven discovery of catalyst genes with application to CO2 activation on semiconductor oxides. Nature Communications, 2022, 13, 419.	12.8	45
25	Two-to-three dimensional transition in neutral gold clusters: The crucial role of van der Waals interactions and temperature. Physical Review Materials, 2019, 3, .	2.4	40
26	Free gold clusters: beyond the static, monostructure description. Faraday Discussions, 2011, 152, 153.	3.2	39
27	Crowd-sourcing materials-science challenges with the NOMAD 2018 Kaggle competition. Npj Computational Materials, 2019, 5, .	8.7	39
28	Efficientab initioschemes for finding thermodynamically stable and metastable atomic structures: benchmark of cascade genetic algorithms. New Journal of Physics, 2014, 16, 123016.	2.9	37
29	Design of kinetic functionals for many-body electron systems: Combining analytical theory with Monte Carlo sampling of electronic configurations. Physical Review B, 2008, 77, .	3.2	35
30	High-pressure diamondlike liquid carbon. Physical Review B, 2004, 69, .	3.2	32
31	Phenol near Ni(111), Ni(110), and Ni(221) surfaces in a vertical ring geometry: A density functional study of the oxygen-surface bonding and O-H cleavage. Physical Review B, 2007, 75, .	3.2	31
32	Computational design of nanoclusters by property-based genetic algorithms: Tuning the electronic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:msub><mml:mi>TiO</mml:mi><mml:mi><mml:r Physical Review B, 2015, 91, .	3.2	29
33	Towards Experimental Handbooks in Catalysis. Topics in Catalysis, 2020, 63, 1683-1699.	2.8	28
34	Trends in the Adsorption and Dissociation of Water Clusters on Flat and Stepped Metallic Surfaces. Journal of Physical Chemistry C, 2014, 118, 29990-29998.	3.1	27
35	Adsorption of alanine on a Ni(111) surface: A multiscale modeling oriented density functional study. Physical Review B, 2006, 74, .	3.2	26
36	Formation of Water Chains on CaO(001): What Drives the 1D Growth?. Journal of Physical Chemistry Letters, 2015, 6, 1204-1208.	4.6	26

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37	Materials genes of heterogeneous catalysis from clean experiments and artificial intelligence. MRS Bulletin, 2021, 46, 1016-1026.	3.5	26
38	Artificial intelligence for high-throughput discovery of topological insulators: The example of alloyed tetradymites. Physical Review Materials, 2020, 4, .	2.4	25
39	Theoretical evidence for unexpected O-rich phases at corners of MgO surfaces. Physical Review Materials, 2017, 1, .	2.4	24
40	Identifying consistent statements about numerical data with dispersion-corrected subgroup discovery. Data Mining and Knowledge Discovery, 2017, 31, 1391-1418.	3.7	23
41	Viewpoint: Atomic-Scale Design Protocols toward Energy, Electronic, Catalysis, and Sensing Applications. Inorganic Chemistry, 2019, 58, 14939-14980.	4.0	23
42	Learning Design Rules for Selective Oxidation Catalysts from High-Throughput Experimentation and Artificial Intelligence. ACS Catalysis, 2022, 12, 2223-2232.	11.2	22
43	Robust recognition and exploratory analysis of crystal structures via Bayesian deep learning. Nature Communications, 2021, 12, 6234.	12.8	20
44	Information-theoretic approach to kinetic-energy functionals: the nearly uniform electron gas. Journal of Mathematical Chemistry, 2010, 48, 78-82.	1.5	17
45	Phosphorus: First principle simulation of a liquidâ€“liquid phase transition. Journal of Chemical Physics, 2005, 122, 184510.	3.0	14
46	Liquid carbon: structure near the freezing line. Journal of Physics Condensed Matter, 2005, 17, S3619-S3624.	1.8	13
47	The interplay between surfaceâ€“water and hydrogen bonding in a water adlayer on Pt(111) and Ag(111). Journal of Physics Condensed Matter, 2007, 19, 242101.	1.8	13
48	Data-driven equation for drugâ€“membrane permeability across drugs and membranes. Journal of Chemical Physics, 2021, 154, 244114.	3.0	13
49	Reaction cycles and poisoning in catalysis by gold clusters: A thermodynamics approach. International Journal of Quantum Chemistry, 2014, 114, 57-65.	2.0	12
50	Strengthening goldâ€“gold bonds by complexing gold clusters with noble gases. Inorganic Chemistry Communication, 2015, 55, 153-156.	3.9	10
51	Identifying Outstanding Transition-Metal-Alloy Heterogeneous Catalysts for the Oxygen Reduction and Evolution Reactions via Subgroup Discovery. Topics in Catalysis, 2022, 65, 196-206.	2.8	10
52	Proton Wires via One-Dimensional Water Chains Adsorbed on Metallic Steps. Journal of Chemical Theory and Computation, 2011, 7, 2681-2684.	5.3	9
53	Electronic energy functionals: Levyâ€“Lieb principle within the ground state path integral quantum Monte Carlo. International Journal of Quantum Chemistry, 2013, 113, 155-160.	2.0	9
54	Determining surface phase diagrams including anharmonic effects. Physical Review B, 2019, 100, .	3.2	9

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55	Structure and Electronic Properties of Transition-Metal/Mg Bimetallic Clusters at Realistic Temperatures and Oxygen Partial Pressures. Journal of Physical Chemistry C, 2018, 122, 16788-16794.	3.1	8
56	(Meta-)stability and Coreâ€“Shell Dynamics of Gold Nanoclusters at Finite Temperature. Journal of Physical Chemistry Letters, 2019, 10, 685-692.	4.6	8
57	SISSO++: A C++ Implementation of the Sure-Independence Screening and Sparsifying Operator Approach. Journal of Open Source Software, 2022, 7, 3960.	4.6	8
58	Trends in atomistic simulation software usage [Article v1.0]. Living Journal of Computational Molecular Science, 2021, 3, .	6.4	7
59	Numerical quality control for DFT-based materials databases. Npj Computational Materials, 2022, 8, .	8.7	6
60	Alkanethiol headgroup on metal (111)-surfaces: general features of the adsorption onto group 10 and 11 transition metals. Journal of Physics Condensed Matter, 2007, 19, 176004.	1.8	5
61	Simulating the phosphorus fluidâ€“liquid phase transition up to the critical point. Journal of Physics Condensed Matter, 2007, 19, 416104.	1.8	5
62	Liquid Carbon: Freezing Line and Structure Near Freezing. Carbon Materials, 2010, , 1-36.	1.2	4
63	Finding predictive models for singlet fission by machine learning. Npj Computational Materials, 2022, 8, .	8.7	4
64	A quantum reactive scattering perspective on electronic nonadiabaticity. European Physical Journal B, 2014, 87, 1.	1.5	2
65	Levy-Lieb-Based Monte Carlo Study of the Dimensionality Behaviour of the Electronic Kinetic Functional. Computation, 2017, 5, 30.	2.0	1
66	AbÂInitio Approach for Thermodynamic Surface Phases with Full Consideration of Anharmonic Effects: The Example of Hydrogen at Si(100). Physical Review Letters, 2022, 128, .	7.8	1
67	Application of (Kohnâ€“Sham) Density-Functional Theory to Real Materials. Letters in Mathematical Physics, 2014, , 191-206.	0.6	0