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	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
2	Learning Design Rules for Selective Oxidation Catalysts from High-Throughput Experimentation and Artificial Intelligence. ACS Catalysis, 2022, 12, 2223-2232.	11.2	22
3	Artificial-intelligence-driven discovery of catalyst genes with application to CO2 activation on semiconductor oxides. Nature Communications, 2022, 13, 419.	12.8	45
4	SISSO++: A C++ Implementation of the Sure-Independence Screening and Sparsifying Operator Approach. Journal of Open Source Software, 2022, 7, 3960.	4.6	8
5	Numerical quality control for DFT-based materials databases. Npj Computational Materials, 2022, 8, .	8.7	6
6	Finding predictive models for singlet fission by machine learning. Npj Computational Materials, 2022, 8, .	8.7	4
7	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
8	Data-driven equation for drugâ€“membrane permeability across drugs and membranes. Journal of Chemical Physics, 2021, 154, 244114.	3.0	13
9	Materials genes of heterogeneous catalysis from clean experiments and artificial intelligence. MRS Bulletin, 2021, 46, 1016-1026.	3.5	26
10	Trends in atomistic simulation software usage [Article v1.0]. Living Journal of Computational Molecular Science, 2021, 3, .	6.4	7
11	Robust recognition and exploratory analysis of crystal structures via Bayesian deep learning. Nature Communications, 2021, 12, 6234.	12.8	20
12	Towards Experimental Handbooks in Catalysis. Topics in Catalysis, 2020, 63, 1683-1699.	2.8	28
13	Identifying domains of applicability of machine learning models for materials science. Nature Communications, 2020, 11, 4428.	12.8	66
14	Artificial intelligence for high-throughput discovery of topological insulators: The example of alloyed tetradymites. Physical Review Materials, 2020, 4, .	2.4	25
15	Viewpoint: Atomic-Scale Design Protocols toward Energy, Electronic, Catalysis, and Sensing Applications. Inorganic Chemistry, 2019, 58, 14939-14980.	4.0	23
16	Determining surface phase diagrams including anharmonic effects. Physical Review B, 2019, 100, .	3.2	9
17	(Meta-)stability and Coreâ€“Shell Dynamics of Gold Nanoclusters at Finite Temperature. Journal of Physical Chemistry Letters, 2019, 10, 685-692.	4.6	8
18	Simultaneous learning of several materials properties from incomplete databases with multi-task SISSO. JPhys Materials, 2019, 2, 024002.	4.2	97

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19	New tolerance factor to predict the stability of perovskite oxides and halides. Science Advances, 2019, 5, eaav0693.	10.3	778
20	Crowd-sourcing materials-science challenges with the NOMAD 2018 Kaggle competition. Npj Computational Materials, 2019, 5, .	8.7	39
21	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
22	GAtor: A First-Principles Genetic Algorithm for Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2018, 14, 2246-2264.	5.3	86
23	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
24	Insightful classification of crystal structures using deep learning. Nature Communications, 2018, 9, 2775.	12.8	237
25	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
26	Learning physical descriptors for materials science by compressed sensing. New Journal of Physics, 2017, 19, 023017.	2.9	100
27	Uncovering structure-property relationships of materials by subgroup discovery. New Journal of Physics, 2017, 19, 013031.	2.9	77
28	Identifying consistent statements about numerical data with dispersion-corrected subgroup discovery. Data Mining and Knowledge Discovery, 2017, 31, 1391-1418.	3.7	23
29	Towards efficient data exchange and sharing for big-data driven materials science: metadata and data formats. Npj Computational Materials, 2017, 3, .	8.7	79
30	Levy-Lieb-Based Monte Carlo Study of the Dimensionality Behaviour of the Electronic Kinetic Functional. Computation, 2017, 5, 30.	2.0	1
31	Theoretical evidence for unexpected O-rich phases at corners of MgO surfaces. Physical Review Materials, 2017, 1, .	2.4	24
32	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
33	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:mn>Physical Review B, 2015, 91, .	3.2	29
34	Big Data of Materials Science: Critical Role of the Descriptor. Physical Review Letters, 2015, 114, 105503.	7.8	658
35	Strengthening goldâ€“gold bonds by complexing gold clusters with noble gases. Inorganic Chemistry Communication, 2015, 55, 153-156.	3.9	10
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	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
38	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
39	Reaction cycles and poisoning in catalysis by gold clusters: A thermodynamics approach. International Journal of Quantum Chemistry, 2014, 114, 57-65.	2.0	12
40	A quantum reactive scattering perspective on electronic nonadiabaticity. European Physical Journal B, 2014, 87, 1.	1.5	2
41	Application of (Kohnâ€“Sham) Density-Functional Theory to Real Materials. Letters in Mathematical Physics, 2014, , 191-206.	0.6	0
42	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
43	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
44	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
45	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
46	Proton Wires via One-Dimensional Water Chains Adsorbed on Metallic Steps. Journal of Chemical Theory and Computation, 2011, 7, 2681-2684.	5.3	9
47	Free gold clusters: beyond the static, monostructure description. Faraday Discussions, 2011, 152, 153.	3.2	39
48	Theory and hierarchical calculations of the structure and energetics of [0001] tilt grain boundaries in graphene. Physical Review B, 2011, 84, .	3.2	84
49	Information-theoretic approach to kinetic-energy functionals: the nearly uniform electron gas. Journal of Mathematical Chemistry, 2010, 48, 78-82.	1.5	17
50	Liquid Carbon: Freezing Line and Structure Near Freezing. Carbon Materials, 2010, , 1-36.	1.2	4
51	Surface-induced crystallization in supercooled tetrahedral liquids. Nature Materials, 2009, 8, 726-730.	27.5	84
52	State-of-the-art models for the phase diagram of carbon and diamond nucleation. Molecular Physics, 2008, 106, 2011-2038.	1.7	58
53	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
54	Phenylalanine near Inorganic Surfaces:Â Conformational Statistics vs Specific Chemistry. Journal of the American Chemical Society, 2008, 130, 2634-2638.	13.7	46

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55	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
56	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
57	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
58	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
59	Simulating the phosphorus fluidâ€“liquid phase transition up to the critical point. Journal of Physics Condensed Matter, 2007, 19, 416104.	1.8	5
60	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
61	Adsorption of alanine on a Ni(111) surface: A multiscale modeling oriented density functional study. Physical Review B, 2006, 74, .	3.2	26
62	Improved long-range reactive bond-order potential for carbon. I. Construction. Physical Review B, 2005, 72, .	3.2	230
63	Phosphorus: First principle simulation of a liquidâ€“liquid phase transition. Journal of Chemical Physics, 2005, 122, 184510.	3.0	14
64	Modeling the Phase Diagram of Carbon. Physical Review Letters, 2005, 94, 145701.	7.8	119
65	Liquid carbon: structure near the freezing line. Journal of Physics Condensed Matter, 2005, 17, S3619-S3624.	1.8	13
66	Improved long-range reactive bond-order potential for carbon. II. Molecular simulation of liquid carbon. Physical Review B, 2005, 72, .	3.2	48
67	High-pressure diamondlike liquid carbon. Physical Review B, 2004, 69, .	3.2	32