Alessandro Curioni

List of Publications by Year
in descending order

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57	4,614	147801	161849
papers	citations	31 h-index	54 g-index

59	59	59	6113
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Thiols and Disulfides on the Au(111) Surface:Â The Headgroupâ˜Gold Interaction. Journal of the American Chemical Society, 2000, 122, 3839-3842.	13.7	591
2	The Chemistry of Water on Alumina Surfaces: Reaction Dynamics from First Principles. , 1998, 282, 265-268.		512
3	Alq3: ab initio calculations of its structural and electronic properties in neutral and charged states. Chemical Physics Letters, 1998, 294, 263-271.	2.6	350
4	Mixed-precision in-memory computing. Nature Electronics, 2018, 1, 246-253.	26.0	315
5	Solid-State Electrolytes: Revealing the Mechanisms of Li-Ion Conduction in Tetragonal and Cubic LLZO by First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 6668-6679.	3.1	176
6	Efficient linear scaling geometry optimization and transition-state search for direct wavefunction optimization schemes in density functional theory using a plane-wave basis. Computational Materials Science, 2003, 27, 437-445.	3.0	172
7	New advances in chemistry and materials science with CPMD and parallel computing. Parallel Computing, 2000, 26, 819-842.	2.1	146
8	The mechanisms underlying the enhanced resolution of atomic force microscopy with functionalized tips. New Journal of Physics, 2010, 12, 125020.	2.9	131
9	Metalâ˜Alq3Complexes:Â The Nature of the Chemical Bonding. Journal of the American Chemical Society, 1999, 121, 8216-8220.	13.7	124
10	Density functional theory approach to thiols and disulfides on gold: Au(111) surface and clusters. International Journal of Quantum Chemistry, 2000, 80, 598-608.	2.0	116
11	Unconventional Bonding of Azafullerenes:Â Theory and Experiment. Journal of the American Chemical Society, 1996, 118, 11335-11336.	13.7	112
12	Billion vortex particle direct numerical simulations of aircraft wakes. Computer Methods in Applied Mechanics and Engineering, 2008, 197, 1296-1304.	6.6	111
13	Freedom and Constraints of a Metal Atom Encapsulated in Fullerene Cages. Physical Review Letters, 1996, 77, 834-837.	7.8	105
14	Car-Parrinello Molecular Dynamics on Massively Parallel Computers. ChemPhysChem, 2005, 6, 1788-1793.	2.1	105
15	Density Functional Theory-Based Molecular Dynamics Simulation of Acid-Catalyzed Chemical Reactions in Liquid Trioxane. Journal of the American Chemical Society, 1997, 119, 7218-7229.	13.7	97
16	Ab initio simulation of the equation of state and kinetics of shocked water. Journal of Chemical Physics, 2009, 130, 124517.	3.0	91
17	Ultrafast transformation of graphite to diamond: An ab initio study of graphite under shock compression. Journal of Chemical Physics, 2008, 128, 184701.	3.0	84
18	Decanethiols on Gold:Â The Structure of Self-Assembled Monolayers Unraveled with Computer Simulations. Langmuir, 2003, 19, 3567-3571.	3.5	83

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19	On-Ball Doping of Fullerenes: The Electronic Structure ofC59N Dimers from Experiment and Theory. Physical Review Letters, 1997, 78, 4249-4252.	7.8	79
20	Mechanisms of Propylene Glycol and Triacetin Pyrolysis. Journal of Physical Chemistry A, 2012, 116, 4602-4609.	2.5	79
21	Image Distortions of a Partially Fluorinated Hydrocarbon Molecule in Atomic Force Microscopy with Carbon Monoxide Terminated Tips. Nano Letters, 2014, 14, 6127-6131.	9.1	73
22	A Revisited Picture of the Mechanism of Glycerol Dehydration. Journal of Physical Chemistry A, 2011, 115, 3592-3595.	2.5	65
23	Dual-level parallelism for ab initio molecular dynamics: Reaching teraflop performance with the CPMD code. Parallel Computing, 2005, 31, 1-17.	2.1	59
24	Structural origin of resistance drift in amorphous GeTe. Physical Review B, 2016, 93, .	3.2	59
25	Why Do Divalent Metal Ions Either Promote or Inhibit Enzymatic Reactions?. Journal of Biological Chemistry, 2003, 278, 4381-4384.	3.4	56
26	Ab initioderived augmented Tersoff potential for silicon oxynitride compounds and their interfaces with silicon. Physical Review B, 2006, 73, .	3.2	54
27	A New Piece in the Puzzle of Lithium/Air Batteries: Computational Study on the Chemical Stability of Propylene Carbonate in the Presence of Lithium Peroxide. Chemistry - A European Journal, 2012, 18, 3510-3520.	3.3	51
28	AbÂInitioDesign of High-kDielectrics:LaxY1â^'xAlO3. Physical Review Letters, 2005, 94, 146401.	7.8	47
29	Metalâ^'Carbon Nanotube Contacts: The Link between Schottky Barrier and Chemical Bonding. Journal of the American Chemical Society, 2008, 130, 5848-5849.	13.7	43
30	A simple model of molecular imaging with noncontact atomic force microscopy. New Journal of Physics, 2012, 14, 083023.	2.9	41
31	Chemisorption on small clusters: can vertical detachment energy measurements provide chemical information? H on Au as a case study. Chemical Physics Letters, 2002, 361, 389-396.	2.6	38
32	Large-Scale Simulations of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>a</mml:mi></mml:math>-Si:H: The Origin of Midgap States Revisited. Physical Review Letters, 2011, 107, 255502.	7.8	32
33	Density-Functional Theory Study of Electronic and Structural Properties of Doped Polypyrroles. Journal of the American Chemical Society, 1998, 120, 4832-4839.	13.7	31
34	Effects of Nitridation on the Characteristics of Silicon Dioxide: Dielectric and Structural Properties fromab initioCalculations. Physical Review Letters, 2004, 92, 236405.	7.8	30
35	Chemical reactivity of aprotic electrolytes on a solid Li₂O₂ surface: screening solvents for Liâ€"air batteries. New Journal of Physics, 2013, 15, 095009.	2.9	30
36	The structure of the SiO2â^•Si(100) interface from a restraint-free search using computer simulations. Applied Physics Letters, 2006, 88, 012101.	3.3	29

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37	Chemical shifts of diamagnetic azafullerenes: (C59N)2 and C59HN. Chemical Physics Letters, 1997, 274, 231-234.	2.6	26
38	Disproving a Silicon Analog of an Alkyne with the Aid of Topological Analyses of the Electronic Structure and Ab Initio Molecular Dynamics Calculations. ChemPhysChem, 2005, 6, 1795-1799.	2.1	26
39	Calculation of nonadiabatic couplings in density-functional theory. Journal of Chemical Physics, 2005, 122, 034105.	3.0	26
40	Density-Functional-Theory-Based Molecular Dynamics Study of 1,3,5-Trioxane and 1,3-Dioxolane Protolysis. Journal of the American Chemical Society, 1994, 116, 11251-11255.	13.7	22
41	Density-Functional Theory and Car-Parinello Study of Electronic, Structural, and Dynamical Properties of the Hexapyrrole Molecule. Journal of Physical Chemistry A, 2000, 104, 8546-8550.	2.5	20
42	Exohedral Hydrogen Chemisorption on a Carbon Nanotube: The Clustering Effect. Journal of Physical Chemistry C, 2012, 116, 269-275.	3.1	18
43	Reactive potential for the study of phase-change materials: GeTe. New Journal of Physics, 2013, 15, 123006.	2.9	18
44	Anomalous Behavior of the Dielectric Constant of Hafnium Silicates: A First Principles Study. Physical Review Letters, 2007, 98, 037602.	7.8	17
45	Computational Study of Lithium Titanate as a Possible Cathode Material for Solid-State Lithiumâ€“Sulfur Batteries. Journal of Physical Chemistry C, 2015, 119, 9681-9691.	3.1	16
46	Reply to Comment on â€œDisproving a Silicon Analog of an Alkyne with the Aid of Topological Analyses of the Electronic Structure and Ab Initio Molecular Dynamics Calculationsâ€• ChemPhysChem, 2006, 7, 801-802.	2.1	15
47	Changing computing paradigms towards power efficiency. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130278.	3.4	15
48	The organicâ€“cathode interface in Alq3-based organic light-emitting devices: new insights from ab-initio molecular dynamics. Synthetic Metals, 2000, 111-112, 299-301.	3.9	13
49	The Elusiveness of Coffee Aroma:Â New Insights from a Non-empirical Approach. Journal of Agricultural and Food Chemistry, 2003, 51, 3092-3096.	5.2	12
50	Shedding Light on Lithium/Air Batteries Using Millions of Threads on the BG/Q Supercomputer. , 2014, , .		11
51	Atomic Oxygen Chemisorption on Carbon Nanotubes Revisited with Theory and Experiment. Journal of Physical Chemistry C, 2013, 117, 1948-1954.	3.1	8
52	Modeling the Impact of Solid Surfaces in Thermal Degradation Processes. ChemPhysChem, 2013, 14, 88-91.	2.1	4
53	Characterizing and Understanding Divalent Adsorbates on Carbon Nanotubes with Ab Initio and Classical Approaches: Size, Chirality, and Coverage Effects. Journal of Chemical Theory and Computation, 2014, 10, 4672-4683.	5.3	4
54	New Scalability Frontiers in Ab Initio Electronic Structure Calculations Using the BG/L Supercomputer. , 2007, , 1026-1035.		2

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55	Towards a Parameter-Free Characterization of Charge Transfer via Hopping: The Case of tris(8-Hydroxyquinolato) Aluminum. Physical Review Letters, 2007, 98, 076803.	7.8	1
56	Vortex Methods for Massively Parallel Computer Architectures. Lecture Notes in Computer Science, 2008, , 479-489.	1.3	0
57	STUDYING THE EFFECTS OF NITROGEN AND HAFNIUM INCORPORATION INTO THE SIO2/SI(100) INTERFACE WITH REPLICA-EXCHANGE MOLECULAR DYNAMICS AND DENSITYFUNCTIONAL- THEORY CALCULATIONS. , 2006, , 203-214.		0