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	Mixed-precision in-memory computing. Nature Electronics, 2018, 1, 246-253.	26.0	315
2	Structural origin of resistance drift in amorphous GeTe. Physical Review B, 2016, 93, .	3.2	59
3	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
4	Changing computing paradigms towards power efficiency. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130278.	3.4	15
5	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
6	Shedding Light on Lithium/Air Batteries Using Millions of Threads on the BG/Q Supercomputer. , 2014, , .		11
7	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
8	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
9	Atomic Oxygen Chemisorption on Carbon Nanotubes Revisited with Theory and Experiment. Journal of Physical Chemistry C, 2013, 117, 1948-1954.	3.1	8
10	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
11	Modeling the Impact of Solid Surfaces in Thermal Degradation Processes. ChemPhysChem, 2013, 14, 88-91.	2.1	4
12	Reactive potential for the study of phase-change materials: GeTe. New Journal of Physics, 2013, 15, 123006.	2.9	18
13	Mechanisms of Propylene Glycol and Triacetin Pyrolysis. Journal of Physical Chemistry A, 2012, 116, 4602-4609.	2.5	79
14	Exohedral Hydrogen Chemisorption on a Carbon Nanotube: The Clustering Effect. Journal of Physical Chemistry C, 2012, 116, 269-275.	3.1	18
15	A simple model of molecular imaging with noncontact atomic force microscopy. New Journal of Physics, 2012, 14, 083023.	2.9	41
16	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
17	A Revisited Picture of the Mechanism of Glycerol Dehydration. Journal of Physical Chemistry A, 2011, 115, 3592-3595.	2.5	65
18	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

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19	The mechanisms underlying the enhanced resolution of atomic force microscopy with functionalized tips. New Journal of Physics, 2010, 12, 125020.	2.9	131
20	Ab initio simulation of the equation of state and kinetics of shocked water. Journal of Chemical Physics, 2009, 130, 124517.	3.0	91
21	Billion vortex particle direct numerical simulations of aircraft wakes. Computer Methods in Applied Mechanics and Engineering, 2008, 197, 1296-1304.	6.6	111
22	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
23	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
24	Vortex Methods for Massively Parallel Computer Architectures. Lecture Notes in Computer Science, 2008, , 479-489.	1.3	0
25	Anomalous Behavior of the Dielectric Constant of Hafnium Silicates: A First Principles Study. Physical Review Letters, 2007, 98, 037602.	7.8	17
26	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
27	New Scalability Frontiers in Ab Initio Electronic Structure Calculations Using the BG/L Supercomputer. , 2007, , 1026-1035.		2
28	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
29	Ab initioderived augmented Tersoff potential for silicon oxynitride compounds and their interfaces with silicon. Physical Review B, 2006, 73, .	3.2	54
30	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
31	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
32	Dual-level parallelism for ab initio molecular dynamics: Reaching teraflop performance with the CPMD code. Parallel Computing, 2005, 31, 1-17.	2.1	59
33	Car-Parrinello Molecular Dynamics on Massively Parallel Computers. ChemPhysChem, 2005, 6, 1788-1793.	2.1	105
34	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
35	Calculation of nonadiabatic couplings in density-functional theory. Journal of Chemical Physics, 2005, 122, 034105.	3.0	26
36	AbÂInitioDesign of High-kDielectrics:LaxY1â"xAlO3. Physical Review Letters, 2005, 94, 146401.	7.8	47

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37	Effects of Nitridation on the Characteristics of Silicon Dioxide: Dielectric and Structural Properties fromab initioCalculations. Physical Review Letters, 2004, 92, 236405.	7.8	30
38	Decanethiols on Gold:Â The Structure of Self-Assembled Monolayers Unraveled with Computer Simulations. Langmuir, 2003, 19, 3567-3571.	3.5	83
39	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
40	Why Do Divalent Metal Ions Either Promote or Inhibit Enzymatic Reactions?. Journal of Biological Chemistry, 2003, 278, 4381-4384.	3.4	56
41	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
42	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
43	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
44	New advances in chemistry and materials science with CPMD and parallel computing. Parallel Computing, 2000, 26, 819-842.	2.1	146
45	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
46	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
47	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
48	Metalâ^'Alq3Complexes:Â The Nature of the Chemical Bonding. Journal of the American Chemical Society, 1999, 121, 8216-8220.	13.7	124
49	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
50	The Chemistry of Water on Alumina Surfaces: Reaction Dynamics from First Principles. , 1998, 282, 265-268.		512
51	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
52	On-Ball Doping of Fullerenes: The Electronic Structure ofC59N Dimers from Experiment and Theory. Physical Review Letters, 1997, 78, 4249-4252.	7.8	79
53	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
54	Chemical shifts of diamagnetic azafullerenes: (C59N)2 and C59HN. Chemical Physics Letters, 1997, 274, 231-234.	2.6	26

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55	Unconventional Bonding of Azafullerenes:Â Theory and Experiment. Journal of the American Chemical Society, 1996, 118, 11335-11336.	13.7	112
56	Freedom and Constraints of a Metal Atom Encapsulated in Fullerene Cages. Physical Review Letters, 1996, 77, 834-837.	7.8	105
57	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