Marco Buongiorno Nardelli

List of Publications by Year
in descending order

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136 papers	15,564 citations	34016 52 h-index	16605 123 g-index
140 all docs	140 docs citations	140 times ranked	17721 citing authors

#	Article	IF	Citations
1	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	0.7	4,303
2	The high-throughput highway to computational materials design. Nature Materials, 2013, 12, 191-201.	13.3	1,475
3	AFLOWLIB.ORG: A distributed materials properties repository from high-throughput ab initio calculations. Computational Materials Science, 2012, 58, 227-235.	1.4	811
4	Convergence of multi-valley bands as the electronic origin of high thermoelectric performance in CoSb3 skutterudites. Nature Materials, 2015, 14, 1223-1228.	13.3	587
5	Brittle and Ductile Behavior in Carbon Nanotubes. Physical Review Letters, 1998, 81, 4656-4659.	2.9	475
6	Electronic transport in extended systems: Application to carbon nanotubes. Physical Review B, 1999, 60, 7828-7833.	1.1	450
7	Mechanism of strain release in carbon nanotubes. Physical Review B, 1998, 57, R4277-R4280.	1.1	441
8	Ab initiotransport properties of nanostructures from maximally localized Wannier functions. Physical Review B, 2004, 69, .	1.1	247
9	A search model for topological insulators with high-throughput robustness descriptors. Nature Materials, 2012, 11, 614-619.	13.3	244
10	The AFLOW standard for high-throughput materials science calculations. Computational Materials Science, 2015, 108, 233-238.	1.4	244
11	Ultimate strength of carbon nanotubes: A theoretical study. Physical Review B, 2002, 65, .	1.1	239
12	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	1.3	236
13	High-throughput computational screening of thermal conductivity, Debye temperature, and GrÃ¼neisen parameter using a quasiharmonic Debye model. Physical Review B, 2014, 90, .	1.1	230
14	Carbon Nanotubeâ^'Metal Cluster Composites:Â A New Road to Chemical Sensors?. Nano Letters, 2005, 5, 847-851.	4.5	209
15	Band Structure and Quantum Conductance of Nanostructures from Maximally Localized Wannier Functions: The Case of Functionalized Carbon Nanotubes. Physical Review Letters, 2005, 95, 076804.	2.9	187
16	Fullerene Coalescence in Nanopeapods:â€‰ A Path to Novel Tubular Carbon. Nano Letters, 2003, 3, 1037-1042.	4.5	185
17	The Interface Phase and the Schottky Barrier for a Crystalline Dielectric on Silicon. Science, 2003, 300, 1726-1730.	6.0	163
18	Mechanical properties, defects and electronic behavior of carbon nanotubes. Carbon, 2000, 38, 1703-1711.	5.4	162

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19	A RESTful API for exchanging materials data in the AFLOWLIB.org consortium. Computational Materials Science, 2014, 93, 178-192.	1.4	148
20	Dissociation of Water on Defective Carbon Substrates. Physical Review Letters, 2005, 95, 136105.	2.9	139
21	Mechanical deformations and coherent transport in carbon nanotubes. Physical Review B, 1999, 60, R16338-R16341.	1.1	137
22	Reformulation of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math>as a Pseudohybrid Hubbard Density Functional for Accelerated Materials Discovery. Physical Review X, 2015, 5, .	2.8	127
23	Polarization field effects on the electron-hole recombination dynamics in In0.2Ga0.8N/In1â^'xGaxN multiple quantum wells. Applied Physics Letters, 1997, 71, 3135-3137.	1.5	125
24	Electronic and field emission properties of boron nitride/carbon nanotube superlattices. Applied Physics Letters, 2002, 81, 46-48.	1.5	118
25	Ab InitioStudies of Polarization and Piezoelectricity in Vinylidene Fluoride and BN-Based Polymers. Physical Review Letters, 2004, 92, 115504.	2.9	116
26	First principles study of the permeability of graphene to hydrogen atoms. Physical Chemistry Chemical Physics, 2013, 15, 16132.	1.3	116
27	O(N)real-space method forab initioquantum transport calculations: Application to carbon nanotubeâ€“metal contacts. Physical Review B, 2001, 64, .	1.1	115
28	Dielectric properties and Raman spectra of ZnO from a first principles finite-differences/finite-fields approach. Scientific Reports, 2013, 3, 2999.	1.6	110
29	Ad-dimers on Strained Carbon Nanotubes: A New Route for Quantum Dot Formation?. Physical Review Letters, 1999, 83, 4132-4135.	2.9	104
30	Tunable Resistance of a Carbon Nanotube-Graphite Interface. , 2000, 290, 1742-1744.		102
31	Strain effects on the interface properties of nitride semiconductors. Physical Review B, 1997, 55, R7323-R7326.	1.1	101
32	Theory of surface morphology of wurtzite GaN (0001) surfaces. Physical Review B, 1997, 56, R12725-R12728.	1.1	100
33	Theoretical STM signatures and transport properties of native defects in carbon nanotubes. Physical Review B, 2000, 61, 14194-14203.	1.1	96
34	Surface polar phonon dominated electron transport in graphene. Applied Physics Letters, 2010, 97, .	1.5	93
35	Lip-Lip Interactions and the Growth of Multiwalled Carbon Nanotubes. Physical Review Letters, 1998, 80, 313-316.	2.9	91
36	Adsorption and catalysis: The effect of confinement on chemical reactions. Applied Surface Science, 2005, 252, 766-777.	3.1	85

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37	Modification of Molecular Spin Crossover in Ultrathin Films. Nano Letters, 2013, 13, 1429-1434.	4.5	83
38	Phase Equilibria in High Energy Density PVDF-Based Polymers. Physical Review Letters, 2007, 99, 047801.	2.9	77
39	Intrinsic electron transport properties of carbon nanotube Y-junctions. Applied Physics Letters, 2002, 81, 5234-5236.	1.5	74
40	PAOFLOW: A utility to construct and operate on ab initio Hamiltonians from the projections of electronic wavefunctions on atomic orbital bases, including characterization of topological materials. Computational Materials Science, 2018, 143, 462-472.	1.4	74
41	First-Principles Theory of Correlated Transport through Nanojunctions. Physical Review Letters, 2005, 94, 116802.	2.9	72
42	Thermoelectric properties of graphene nanoribbons, junctions and superlattices. Journal of Physics Condensed Matter, 2010, 22, 372202.	0.7	72
43	AFLOWÏ€: A minimalist approach to high-throughput ab initio calculations including the generation of tight-binding hamiltonians. Computational Materials Science, 2017, 136, 76-84.	1.4	70
44	Iron(ii) spin crossover films on Au(111): scanning probe microscopy and photoelectron spectroscopy. Chemical Communications, 2013, 49, 10446.	2.2	69
45	Dynamic Conductance of Carbon Nanotubes. Physical Review Letters, 2000, 84, 2921-2924.	2.9	67
46	Ab initiocorrelation effects on the electronic and transport properties of metal(II)-phthalocyanine-based devices. Nanotechnology, 2007, 18, 424013.	1.3	65
47	An efficient and accurate framework for calculating lattice thermal conductivity of solids: AFLOWâ€"AAPL Automatic Anharmonic Phonon Library. Npj Computational Materials, 2017, 3, .	3.5	65
48	Effective and accurate representation of extended Bloch states on finite Hilbert spaces. Physical Review B, 2013, 88, .	1.1	64
49	Band Engineering and Magnetic Doping of Epitaxial Graphene on SiC (0001). Physical Review Letters, 2010, 104, 146801.	2.9	63
50	Room-temperature ferroelectric switching of spin-to-charge conversion in germanium telluride. Nature Electronics, 2021, 4, 740-747.	13.1	62
51	Electronic and Transport Properties of Artificial Gold Chains. Physical Review Letters, 2004, 93, 096404.	2.9	56
52	Improved predictions of the physical properties of Zn- and Cd-based wide band-gap semiconductors: A validation of the ACBN0 functional. Physical Review B, 2015, 91, .	1.1	56
53	AFLUX: The LUX materials search API for the AFLOW data repositories. Computational Materials Science, 2017, 137, 362-370.	1.4	56
54	High-throughput prediction of finite-temperature properties using the quasi-harmonic approximation. Computational Materials Science, 2016, 125, 82-91.	1.4	51

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55	Combining the AFLOW GIBBS and elastic libraries to efficiently and robustly screen thermomechanical properties of solids. Physical Review Materials, 2017, 1, .	0.9	47
56	Phonon engineering in nanostructures: Controlling interfacial thermal resistance in multilayer-graphene/dielectric heterojunctions. Applied Physics Letters, 2012, 101, 113111.	1.5	46
57	CO Adsorption on Noble Metal Clusters: Local Environment Effects. Journal of Physical Chemistry C, 2011, 115, 5637-5647.	1.5	45
58	Toward Realistic Amorphous Topological Insulators. Nano Letters, 2019, 19, 8941-8946.	4.5	44
59	Electric Field Induced Phase Transitions in Polymers: A Novel Mechanism for High Speed Energy Storage. Physical Review Letters, 2012, 108, 087802.	2.9	43
60	Accurate tight-binding Hamiltonian matrices fromab initiocalculations: Minimal basis sets. Physical Review B, 2016, 93, .	1.1	43
61	Complex Materials for Molecular Spintronics Applications: Cobalt Bis(dioxolene) Valence Tautomers, from Molecules to Polymers. Journal of Physical Chemistry B, 2012, 116, 13141-13148.	1.2	42
62	Confinement effects on chemical reactionsâ€"Toward an integrated rational catalyst design. Applied Surface Science, 2007, 253, 5570-5579.	3.1	40
63	Accurate tight-binding Hamiltonians for two-dimensional and layered materials. Physical Review B, 2016, 93, .	1.1	40
64	High throughput combinatorial method for fast and robust prediction of lattice thermal conductivity. Scripta Materialia, 2017, 129, 88-93.	2.6	40
65	Coordination corrected ab initio formation enthalpies. Npj Computational Materials, 2019, 5, .	3.5	38
66	Hydrogen Adsorption on Platinumâ€"Gold Bimetallic Nanoparticles: A Density Functional Theory Study. Journal of Physical Chemistry C, 2013, 117, 15050-15060.	1.5	36
67	Charge transfer equilibria in ambient-exposed epitaxial graphene on (0001Â¯) 6â€‰H-SiC. Journal of Applied Physics, 2012, 111, 113706.	1.1	35
68	Catalytic role of carbons in methane decomposition for CO- and CO2-free hydrogen generation. Journal of Chemical Physics, 2008, 128, 214702.	1.2	34
69	Giant spin Hall effect in two-dimensional monochalcogenides. 2D Materials, 2019, 6, 025012.	2.0	30
70	Role of quantum confinement and interlayer coupling in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">CrI</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> -graphene magnetic tunnel junctions. Physical Review B, 2020, 101, .	1.1	29
71	Effect of Confinement on Chemical Reactions. Adsorption, 2005, 11, 349-354.	1.4	28
72	Improved electronic structure and magnetic exchange interactions in transition metal oxides. Journal of Physics Condensed Matter, 2017, 29, 444003.	0.7	28

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73	Phonon softening and high-pressure low-symmetry phases of cesium iodide. Physical Review Letters, 1992, 69, 1069-1072.	2.9	27
74	Systematic Band Gap Tuning of BaSnO₃ via Chemical Substitutions: The Role of Clustering in Mixed-Valence Perovskites. Chemistry of Materials, 2017, 29, 9378-9385.	3.2	27
75	Chemisorption of H on GaAs(110): a First-Principles Calculation. Europhysics Letters, 1990, 13, 653-658.	0.7	26
76	Ordering of a prototypical conjugated molecular system during monolayer growth on the (1Ã—2)-Au(110) surface. Physical Review B, 1996, 53, 1095-1098.	1.1	26
77	First-principles theory of metal-alkaline earth oxide interfaces. Physical Review B, 2006, 73, .	1.1	26
78	Spin Hall effect in prototype Rashba ferroelectrics GeTe and SnTe. Npj Computational Materials, 2020, 6, .	3.5	26
79	Mixed finite element-tight-binding electromechanical analysis of carbon nanotubes. Journal of Applied Physics, 2004, 96, 6756-6760.	1.1	25
80	A remarkable shape-catalytic effect of confinement on the rotational isomerization of small hydrocarbons. Journal of Chemical Physics, 2008, 128, 034704.	1.2	25
81	Accurateab initiotight-binding Hamiltonians: Effective tools for electronic transport and optical spectroscopy from first principles. Physical Review B, 2016, 94, .	1.1	25
82	Ultrathin SnTe films as a route towards all-in-one spintronics devices. 2D Materials, 2020, 7, 025026.	2.0	24
83	High-pressure low-symmetry phases of cesium halides. Physical Review B, 1995, 51, 8060-8068.	1.1	23
84	Real-space multigrid methods for large-scale electronic structure problems. International Journal of Quantum Chemistry, 1997, 65, 531-543.	1.0	22
85	First principles theory of artificial metal chains on NiAl(110) surface. Physical Review B, 2005, 72, .	1.1	22
86	Advanced modeling of materials with PAOFLOW 2.0: New features and software design. Computational Materials Science, 2021, 200, 110828.	1.4	21
87	Molecular design of photoactive acenes for organic photovoltaics. Journal of Chemical Physics, 2009, 130, 194701.	1.2	19
88	Ti-decorated C60 as catalyst for hydrogen generation and storage. Applied Physics Letters, 2010, 96, .	1.5	18
89	Effect of confinement by porous carbons on the unimolecular decomposition of formaldehyde. Journal of Chemical Physics, 2006, 125, 084711.	1.2	17
90	Ab initiothermal transport properties of nanostructures from density functional perturbation theory. Journal of Physics Condensed Matter, 2012, 24, 492204.	0.7	17

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91	FORMATION AND PROPERTIES OF ASTROPHYSICAL CARBONACEOUS DUST. I. AB-INITIO CALCULATIONS OF THE CONFIGURATION AND BINDING ENERGIES OF SMALL CARBON CLUSTERS. Astrophysical Journal, 2015, 800, 30.	1.6	17
92	Unconventional co-existence of plasmon and thermoelectric activity in In:ZnO nanowires. RSC Advances, 2015, 5, 44865-44872.	1.7	16
93	Effects of end group functionalization and level alignment on electron transport in molecular devices. Journal of Chemical Physics, 2008, 128, 024708.	1.2	15
94	Discovery of higher-order topological insulators using the spin Hall conductivity as a topology signature. Npj Computational Materials, 2021, 7, .	3.5	15
95	Theoretical bounds for multiwalled carbon nanotube growth. Chemical Physics Letters, 1998, 296, 471-476.	1.2	14
96	Chiral Steering of Molecular Organization in the Limit of Weak Adsorbateâ^'Substrate Interactions: Enantiopure and Racemic Tartaric Acid Domains on Ag(111). Journal of Physical Chemistry C, 2010, 114, 8917-8925.	1.5	14
97	Substrate-Mediated Intermolecular Hybridization in Binary Phthalocyanine Superstructures. Journal of Physical Chemistry C, 2010, 114, 1041-1045.	1.5	14
98	Dissociation of water over Ti-decorated C60. Journal of Chemical Physics, 2010, 133, 084510.	1.2	13
99	First principles thermodynamical modeling of the binodal and spinodal curves in lead chalcogenides. Physical Chemistry Chemical Physics, 2016, 18, 5005-5011.	1.3	13
100	Quantum computation of silicon electronic band structure. Physical Chemistry Chemical Physics, 2020, 22, 21816-21822.	1.3	13
101	A density-functional study of van der Waals forces: He interaction with a semiconductor surface. Solid State Communications, 1996, 97, 215-219.	0.9	12
102	Activation of water on the TiO2 (110) surface: The case of Ti adatoms. Journal of Chemical Physics, 2012, 136, 064703.	1.2	12
103	First principles study of the optical emission of cadmium yellow: Role of cadmium vacancies. AIP Advances, 2018, 8, .	0.6	12
104	Finite difference methods for ab initio electronic structure and quantum transport calculations of nanostructures. Handbook of Numerical Analysis, 2003, 10, 571-612.	0.9	10
105	Controlling Topological States in Topological/Normal Insulator Heterostructures. ACS Omega, 2018, 3, 15900-15906.	1.6	10
106	Absorption and emission modulation in a MoS₂â€“GaN (0001) heterostructure by interface phononâ€“exciton coupling. Photonics Research, 2019, 7, 1511.	3.4	10
107	Theory of interfaces and surfaces in wide-gap nitrides. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1997, 15, 1144.	1.6	9
108	Atomistic simulations of aromatic polyurea and polyamide for capacitive energy storage. Physical Review B, 2015, 92, .	1.1	9

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109	The Maximum Edge Weight Clique Problem: Formulations and Solution Approaches. Springer Optimization and Its Applications, 2017, , 217-237.	0.6	9
110	The AFLOW Fleet for Materials Discovery. , 2018, , 1-28.		9
111	Thermoelectric Properties of Minerals with the Mawsonite Structure. ACS Applied Energy Materials, 2019, 2, 8068-8078.	2.5	9
112	Mechanical Properties of Chemically Modified Clay. Scientific Reports, 2019, 9, 13698.	1.6	9
113	Vibrational spectral fingerprinting for chemical recognition of biominerals. ChemPhysChem, 2020, 21, 770-778.	1.0	9
114	Relaxation time approximations in PAOFLOW 2.0. Scientific Reports, 2022, 12, 4993.	1.6	9
115	Spinodal Superlattices of Topological Insulators. Chemistry of Materials, 2018, 30, 2331-2340.	3.2	8
116	AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties of solids. Physical Review Materials, 2019, 3, .	0.9	8
117	First-principles simulations of PVDF copolymers with high dielectric energy density: PVDF-HFP and PVDF-BTFE. Physical Review B, 2016, 94, .	1.1	7
118	Hyperbolic Metamaterials with Extreme Mechanical Hardness. Advanced Optical Materials, 2021, 9, 2001904.	3.6	6
119	Isomerization kinetics of small hydrocarbons in confinement. Adsorption, 2008, 14, 181-188.	1.4	5
120	Sequestration and selective oxidation of carbon monoxide on graphene edges. Journal of Physics Condensed Matter, 2009, 21, 355008.	0.7	5
121	The AFLOW Fleet for Materials Discovery. , 2020, , 1785-1812.		4
122	A systematic variational approach to band theory in a quantum computer. RSC Advances, 2021, 11, 39438-39449.	1.7	4
123	Response to â€œComment on â€˜Intrinsic electron transport properties of carbon nanotube Y junctionsâ€™â€Šâ€• [Appl. Phys. Lett. 83, 1674 (2003)]. Applied Physics Letters, 2003, 83, 1676-1677.	1.5	3
124	Topology of Networks in Generalized Musical Spaces. Leonardo Music Journal, 2020, 30, 38-43.	0.1	3
125	Theory of Interfaces and Surfaces of Wide-Gap Nitrides. Materials Research Society Symposia Proceedings, 1997, 482, 904.	0.1	2
126	Rational computational design of optimal catalytic surfaces. Applied Physics Letters, 2010, 97, 233108.	1.5	2

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127	Optical Enhancement in Heteroleptic Ru(II) Polypyridyl Complexes Using Electron-Donor Ancillary Ligands. Journal of Physical Chemistry C, 2014, 118, 8747-8755.	1.5	2
128	Leonardo Gallery: Scientific Delirium Madness 4.0. Leonardo, 2018, 51, 227-238.	0.2	2
129	Networks of materials: Construction and structural analysis. AICHE Journal, 2021, 67, e17051.	1.8	2
130	Two-Layer High-Throughput: Effective Mass Calculations Including Warping. Engineering, 2022, 10, 74-80.	3.2	2
131	High-Throughput Computational Search for Half-Metallic Oxides. Molecules, 2020, 25, 2010.	1.7	1
132	MUSICNTWRK: Data Tools for Music Theory, Analysis and Composition. Lecture Notes in Computer Science, 2021, , 190-215.	1.0	1
133	Tonal harmony and the topology of dynamical score networks. Journal of Mathematics and Music, 2023, 17, 198-212.	0.3	1
134	Quantum algorithm for electronic band structures with local tight-binding orbitals. Scientific Reports, 2022, 12, .	1.6	1
135	Field Emission Properties of BN/C and BN@C Hybrid Nanotubes. Materials Research Society Symposia Proceedings, 2002, 739, 571.	0.1	0
136	The AFLOW Fleet for Materials Discovery. , 2019, , 1-28.		0