Nicola Marzari

List of Publications by Year
in descending order

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264 papers	61,664 citations	6592 79 h-index	849 244 g-index
275 all docs	275 docs citations	275 times ranked	45196 citing authors

#	Article	IF	Citations
1	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	0.7	18,183
2	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	0.7	4,303
3	Maximally localized generalized Wannier functions for composite energy bands. Physical Review B, 1997, 56, 12847-12865.	1.1	3,642
4	wannier90: A tool for obtaining maximally-localised Wannier functions. Computer Physics Communications, 2008, 178, 685-699.	3.0	2,947
5	Maximally localized Wannier functions: Theory and applications. Reviews of Modern Physics, 2012, 84, 1419-1475.	16.4	2,159
6	Uniaxial strain in graphene by Raman spectroscopy:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>G</mml:mi></mml:math>peak splitting, GrÃ¼neisen parameters, and sample orientation. Physical Review B, 2009, 79, .	1.1	1,662
7	An updated version of wannier90: A tool for obtaining maximally-localised Wannier functions. Computer Physics Communications, 2014, 185, 2309-2310.	3.0	1,561
8	Maximally localized Wannier functions for entangled energy bands. Physical Review B, 2001, 65, .	1.1	1,546
9	Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. Nature Nanotechnology, 2018, 13, 246-252.	15.6	1,317
10	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
11	First-principles determination of the structural, vibrational and thermodynamic properties of diamond, graphite, and derivatives. Physical Review B, 2005, 71, .	1.1	955
12	Thermal Contraction and Disordering of the Al(110) Surface. Physical Review Letters, 1999, 82, 3296-3299.	2.9	929
13	Wannier90 as a community code: new features and applications. Journal of Physics Condensed Matter, 2020, 32, 165902.	0.7	807
14	Q<scp>uantum</scp> ESPRESSO toward the exascale. Journal of Chemical Physics, 2020, 152, 154105.	1.2	796
15	Large-Area Epitaxial Monolayer MoS₂. ACS Nano, 2015, 9, 4611-4620.	7.3	712
16	The shear mode of multilayer graphene. Nature Materials, 2012, 11, 294-300.	13.3	568
17	Density Functional Theory in Transition-Metal Chemistry: A Self-Consistent HubbardUApproach. Physical Review Letters, 2006, 97, 103001.	2.9	526
18	Thermal Conductivity of Graphene and Graphite: Collective Excitations and Mean Free Paths. Nano Letters, 2014, 14, 6109-6114.	4.5	449

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19	Surface energies, work functions, and surface relaxations of low-index metallic surfaces from first principles. Physical Review B, 2009, 80, .	1.1	407
20	Role of Disorder and Anharmonicity in the Thermal Conductivity of Silicon-Germanium Alloys: A First-Principles Study. Physical Review Letters, 2011, 106, 045901.	2.9	404
21	AiiDA: automated interactive infrastructure and database for computational science. Computational Materials Science, 2016, 111, 218-230.	1.4	399
22	Phonon Anharmonicities in Graphite and Graphene. Physical Review Letters, 2007, 99, 176802.	2.9	391
23	Precision and efficiency in solid-state pseudopotential calculations. Npj Computational Materials, 2018, 4, .	3.5	390
24	Phonon hydrodynamics in two-dimensional materials. Nature Communications, 2015, 6, 6400.	5.8	385
25	Revised self-consistent continuum solvation in electronic-structure calculations. Journal of Chemical Physics, 2012, 136, 064102.	1.2	383
26	Maximally-localized Wannier functions for disordered systems: Application to amorphous silicon. Solid State Communications, 1998, 107, 7-11.	0.9	363
27	Ensemble Density-Functional Theory forAb InitioMolecular Dynamics of Metals and Finite-Temperature Insulators. Physical Review Letters, 1997, 79, 1337-1340.	2.9	345
28	Electrochemical Windows of Room-Temperature Ionic Liquids from Molecular Dynamics and Density Functional Theory Calculations. Chemistry of Materials, 2011, 23, 2979-2986.	3.2	337
29	Production and processing of graphene and related materials. 2D Materials, 2020, 7, 022001.	2.0	333
30	Self-assembled quantum dots in a nanowire system for quantum photonics. Nature Materials, 2013, 12, 439-444.	13.3	306
31	Exponential Localization of Wannier Functions in Insulators. Physical Review Letters, 2007, 98, 046402.	2.9	297
32	Performance of arsenene and antimonene double-gate MOSFETs from first principles. Nature Communications, 2016, 7, 12585.	5.8	278
33	Surface Composition Tuning of Auâ€“Pt Bimetallic Nanoparticles for Enhanced Carbon Monoxide and Methanol Electro-oxidation. Journal of the American Chemical Society, 2013, 135, 7985-7991.	6.6	266
34	Oxygen Evolution Reaction on La_{1â€“x}Sr_xCoO₃ Perovskites: A Combined Experimental and Theoretical Study of Their Structural, Electronic, and Electrochemical Properties. Chemistry of Materials, 2015, 27, 7662-7672.	3.2	259
35	Unified theory of thermal transport in crystals and glasses. Nature Physics, 2019, 15, 809-813.	6.5	255
36	Potential-induced nanoclustering of metallic catalysts during electrochemical CO2 reduction. Nature Communications, 2018, 9, 3117.	5.8	253

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37	Ab initiotransport properties of nanostructures from maximally localized Wannier functions. Physical Review B, 2004, 69, .	1.1	247
38	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	1.3	236
39	Ultraviolet Photodetectors Based on Anodic TiO₂ Nanotube Arrays. Journal of Physical Chemistry C, 2010, 114, 10725-10729.	1.5	230
40	Sensing Mechanisms for Carbon Nanotube Based NH₃ Gas Detection. Nano Letters, 2009, 9, 1626-1630.	4.5	223
41	BoltzWann: A code for the evaluation of thermoelectric and electronic transport properties with a maximally-localized Wannier functions basis. Computer Physics Communications, 2014, 185, 422-429.	3.0	219
42	Static Dielectric Properties of Carbon Nanotubes from First Principles. Physical Review Letters, 2006, 96, 166801.	2.9	214
43	Koopmansâ€™ condition for density-functional theory. Physical Review B, 2010, 82, .	1.1	206
44	Hubbard parameters from density-functional perturbation theory. Physical Review B, 2018, 98, .	1.1	194
45	Static and dynamical properties of heavy water at ambient conditions from first-principles molecular dynamics. Journal of Chemical Physics, 2005, 122, 204510.	1.2	191
46	Materials Cloud, a platform for open computational science. Scientific Data, 2020, 7, 299.	2.4	189
47	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
48	Acoustic Phonon Lifetimes and Thermal Transport in Free-Standing and Strained Graphene. Nano Letters, 2012, 12, 2673-2678.	4.5	178
49	Achieving DFT accuracy with a machine-learning interatomic potential: Thermomechanics and defects in bcc ferromagnetic iron. Physical Review Materials, 2018, 2, .	0.9	175
50	Highly Active and Stable Iridium Pyrochlores for Oxygen Evolution Reaction. Chemistry of Materials, 2017, 29, 5182-5191.	3.2	172
51	An In Situ Surface-Enhanced Infrared Absorption Spectroscopy Study of Electrochemical CO₂ Reduction: Selectivity Dependence on Surface C-Bound and O-Bound Reaction Intermediates. Journal of Physical Chemistry C, 2019, 123, 5951-5963.	1.5	172
52	Electronâ€“Phonon Interactions and the Intrinsic Electrical Resistivity of Graphene. Nano Letters, 2014, 14, 1113-1119.	4.5	149
53	AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance. Scientific Data, 2020, 7, 300.	2.4	142
54	The Electronic Thermal Conductivity of Graphene. Nano Letters, 2016, 16, 2439-2443.	4.5	137

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55	Cycloaddition Functionalizations to Preserve or Control the Conductance of Carbon Nanotubes. Physical Review Letters, 2006, 97, 116801.	2.9	133
56	Simulation of Heme Using DFT + U:Â A Step toward Accurate Spin-State Energetics. Journal of Physical Chemistry B, 2007, 111, 7384-7391.	1.2	127
57	Breakdown of Optical Phononsâ€™ Splitting in Two-Dimensional Materials. Nano Letters, 2017, 17, 3758-3763.	4.5	127
58	Equipartition of Energy Defines the Sizeâ€“Thickness Relationship in Liquid-Exfoliated Nanosheets. ACS Nano, 2019, 13, 7050-7061.	7.3	123
59	Bandâ€Like Electron Transport with Recordâ€High Mobility in the TCNQ Family. Advanced Materials, 2015, 27, 2453-2458.	11.1	122
60	Grand canonical simulations of electrochemical interfaces in implicit solvation models. Journal of Chemical Physics, 2019, 150, 041730.	1.2	122
61	Electrostatics in periodic boundary conditions and real-space corrections. Physical Review B, 2008, 77, .	1.1	116
62	Unraveling Thermodynamics, Stability, and Oxygen Evolution Activity of Strontium Ruthenium Perovskite Oxide. ACS Catalysis, 2017, 7, 3245-3256.	5.5	113
63	A unified electrostatic and cavitation model for first-principles molecular dynamics in solution. Journal of Chemical Physics, 2006, 124, 074103.	1.2	109
64	The role of nanostructure in the wetting behavior of mixed-monolayer-protected metal nanoparticles. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 9886-9891.	3.3	106
65	Phonon-limited resistivity of graphene by first-principles calculations: Electron-phonon interactions, strain-induced gauge field, and Boltzmann equation. Physical Review B, 2014, 90, .	1.1	105
66	Large-scale synthesis of crystalline g-C ₃ N ₄ nanosheets and high-temperature H ₂ sieving from assembled films. Science Advances, 2020, 6, eaay9851.	4.7	105
67	Spin Channels in Functionalized Graphene Nanoribbons. Nano Letters, 2009, 9, 3425-3429.	4.5	103
68	Defect ordering and defectâ€“domain-wall interactions in PbTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>: A first-principles study. Physical Review B, 2013, 88, .	1.1	100
69	Electronic-structure methods for materials design. Nature Materials, 2021, 20, 736-749.	13.3	96
70	Photoinduced oxidation of carbon nanotubes. Journal of Physics Condensed Matter, 2003, 15, 5915-5921.	0.7	95
71	Mobility of two-dimensional materials from first principles in an accurate and automated framework. Physical Review Materials, 2018, 2, .	0.9	93
72	Self-consistent continuum solvation (SCCS): The case of charged systems. Journal of Chemical Physics, 2013, 139, 214110.	1.2	90

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73	A generalized Poisson and Poisson-Boltzmann solver for electrostatic environments. Journal of Chemical Physics, 2016, 144, 014103.	1.2	88
74	Systematic study of first-row transition-metal diatomic molecules: A self-consistent DFT+U approach. Journal of Chemical Physics, 2010, 133, 114103.	1.2	87
75	Spatially Extended Kondo State in Magnetic Molecules Induced by Interfacial Charge Transfer. Physical Review Letters, 2010, 105, 106601.	2.9	86
76	Ionic correlations and failure of Nernst-Einstein relation in solid-state electrolytes. Physical Review Materials, 2017, 1, .	0.9	86
77	Berry phase and pseudospin winding number in bilayer graphene. Physical Review B, 2011, 84, .	1.1	85
78	Emergence of One-Dimensional Wires of Free Carriers in Transition-Metal-Dichalcogenide Nanostructures. Nano Letters, 2015, 15, 6229-6238.	4.5	85
79	Self-consistent Hubbard parameters from density-functional perturbation theory in the ultrasoft and projector-augmented wave formulations. Physical Review B, 2021, 103, .	1.1	84
80	High Thermal Conductivity in Short-Period Superlattices. Nano Letters, 2011, 11, 5135-5141.	4.5	81
81	Koopmans-compliant functionals and their performance against reference molecular data. Physical Review B, 2014, 90, .	1.1	81
82	High-throughput computational screening for solid-state Li-ion conductors. Energy and Environmental Science, 2020, 13, 928-948.	15.6	80
83	Dielectric response of oxides in the weighted density approximation. Physical Review B, 2000, 62, 12724-12729.	1.1	79
84	Prediction of a Large-Gap and Switchable Kane-Mele Quantum Spin Hall Insulator. Physical Review Letters, 2018, 120, 117701.	2.9	79
85	Soft-Sphere Continuum Solvation in Electronic-Structure Calculations. Journal of Chemical Theory and Computation, 2017, 13, 3829-3845.	2.3	76
86	Evidence of Large Polarons in Photoemission Band Mapping of the Perovskite Semiconductor <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>CsPbBr</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow> Physical Review Letters, 2020, 124, 206402.	2.9	74
87	A self-consistent Hubbard U density-functional theory approach to the addition-elimination reactions of hydrocarbons on bare FeO+. Journal of Chemical Physics, 2008, 129, 134314.	1.2	72
88	Thermal Transport in Crystals as a Kinetic Theory of Relaxons. Physical Review X, 2016, 6, .	2.8	72
89	Ï€-Stacking in Thiophene Oligomers as the Driving Force for Electroactive Materials and Devices. Journal of the American Chemical Society, 2005, 127, 3207-3212.	6.6	71
90	Electrostatics of solvated systems in periodic boundary conditions. Physical Review B, 2014, 90, .	1.1	71

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91	Sliding Mechanisms in Aluminum Grain Boundaries. Physical Review Letters, 1997, 79, 869-872.	2.9	70
92	Proton dynamics in superprotonicCsHSO4. Physical Review B, 2007, 76, .	1.1	69
93	Playing quantum hide-and-seek with the muon: localizing muon stopping sites. Physica Scripta, 2013, 88, 068510.	1.2	67
94	Effects of filling in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CoSb</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:m Local structure, band gap, and phonons from first principles. Physical Review B, 2010, 81, .	3.1	66
95	Accurate potential energy surfaces with a DFT+$U(mathbf {R})$U(R) approach. Journal of Chemical Physics, 2011, 135, 194105.	1.2	63
96	Screw dislocation structure and mobility in body centered cubic Fe predicted by a Gaussian Approximation Potential. Npj Computational Materials, 2018, 4, .	3.5	63
97	Highly Active Nanoperovskite Catalysts for Oxygen Evolution Reaction: Insights into Activity and Stability of Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{2+Î´} and PrBaCo₂O_{5+Î´}. Advanced Functional Materials, 2018, 28, 1804355.	7.8	63
98	Workflows in AiiDA: Engineering a high-throughput, event-based engine for robust and modular computational workflows. Computational Materials Science, 2021, 187, 110086.	1.4	63
99	Structure and phase stability ofGaxIn1â^'xP solid solutions from computational alchemy. Physical Review Letters, 1994, 72, 4001-4004.	2.9	61
100	Improving the Electrical Conductivity of Carbon Nanotube Networks: A First-Principles Study. ACS Nano, 2011, 5, 9726-9736.	7.3	61
101	Realistic Quantitative Descriptions of Electron Transfer Reactions: Diabatic Free-Energy Surfaces from First-Principles Molecular Dynamics. Physical Review Letters, 2006, 97, 028303.	2.9	58
102	First-Principles Prediction of the Equilibrium Shape of Nanoparticles Under Realistic Electrochemical Conditions. Physical Review Letters, 2013, 110, 086104.	2.9	57
103	Quantum states of muons in fluorides. Physical Review B, 2013, 87, .	1.1	57
104	Continuum models of the electrochemical diffuse layer in electronic-structure calculations. Journal of Chemical Physics, 2019, 150, 041722.	1.2	57
105	Ï€-Stacking in Charged Thiophene Oligomers. Journal of Physical Chemistry B, 2004, 108, 17791-17795.	1.2	56
106	An Open-Source Multiscale Framework for the Simulation of Nanoscale Devices. IEEE Transactions on Electron Devices, 2014, 61, 48-53.	1.6	56
107	2-D Materials for Ultrascaled Field-Effect Transistors: One Hundred Candidates under the Ab Initio Microscope. ACS Nano, 2020, 14, 8605-8615.	7.3	56
108	Transition-metal dioxides: A case for the intersite term in Hubbard-model functionals. Journal of Chemical Physics, 2011, 134, 094103.	1.2	55

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109	A converse approach to the calculation of NMR shielding tensors. Journal of Chemical Physics, 2009, 131, 101101.	1.2	54
110	Textural and Micromorphological Effects on the Overall Elastic Response of Macroscopically Anisotropic Composites. Journal of Applied Mechanics, Transactions ASME, 1992, 59, 269-275.	1.1	51
111	Spin and orbital magnetic response in metals: Susceptibility and NMR shifts. Physical Review B, 2007, 76, .	1.1	51
112	First-Principles Study of Non-heme Fe(II) Halogenase SyrB2 Reactivity. Journal of the American Chemical Society, 2009, 131, 14426-14433.	6.6	50
113	Relative Abundance of Z2 Topological Order in Exfoliable Two-Dimensional Insulators. Nano Letters, 2019, 19, 8431-8440.	4.5	50
114	Self-consistent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi><mml:r study of oxygen vacancies in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review Research, 2020, 2, .	1.3	50
115	Electrosorption at metal surfaces from first principles. Npj Computational Materials, 2020, 6, .	3.5	49
116	OPTIMADE, an API for exchanging materials data. Scientific Data, 2021, 8, 217.	2.4	49
117	Absolute band alignment at semiconductor-water interfaces using explicit and implicit descriptions for liquid water. Npj Computational Materials, 2019, 5, .	3.5	48
118	First-principles predictions of Hall and drift mobilities in semiconductors. Physical Review Research, 2021, 3, .	1.3	48
119	Enhanced Electron-Phonon Interaction in Multivalley Materials. Physical Review X, 2019, 9, .	2.8	47
120	Insight into gallium behavior in aluminum grain boundaries from calculation on Î£=11 (113) boundary. Acta Materialia, 2000, 48, 3623-3632.	3.8	46
121	Enhanced Proton Conductivity in Yâ€Doped BaZrO₃ via Strain Engineering. Advanced Science, 2017, 4, 1700467.	5.6	45
122	Gate modulation in carbon nanotube field effect transistors-based NH3 gas sensors. Sensors and Actuators B: Chemical, 2008, 132, 191-195.	4.0	43
123	Engineering polar discontinuities in honeycomb lattices. Nature Communications, 2014, 5, 5157.	5.8	43
124	Solvent-Aware Interfaces in Continuum Solvation. Journal of Chemical Theory and Computation, 2019, 15, 1996-2009.	2.3	43
125	Hubbard-corrected density functional perturbation theory with ultrasoft pseudopotentials. Physical Review B, 2020, 101, .	1.1	43
126	Hydrogen bonding and coordination in normal and supercritical water from x-ray inelastic scattering. Physical Review B, 2007, 76, .	1.1	42

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127	Bulk aluminum at high pressure: A first-principles study. Physical Review B, 2008, 77, .	1.1	42
128	Electronic-Enthalpy Functional for Finite Systems Under Pressure. Physical Review Letters, 2005, 94, 145501.	2.9	41
129	Local Effects in the X-ray Absorption Spectrum of Salt Water. Journal of Physical Chemistry B, 2010, 114, 9594-9601.	1.2	41
130	Rippling ultrafast dynamics of suspended 2D monolayers, graphene. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E6555-E6561.	3.3	41
131	Vibrational Recognition of Adsorption Sites for CO on Platinum and Platinumâ˜Ruthenium Surfaces. Journal of the American Chemical Society, 2007, 129, 11045-11052.	6.6	40
132	Thermoelastic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math>-iron from first-principles. Physical Review B, 2015, 91, .	1.1	40
133	Bulk and Surface Electronic Structure of the Dual-Topology Semimetal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Pt</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow> Physical Review Letters, 2020, 124, 106402.	2.9	40
134	AiiDAlab â€“ an ecosystem for developing, executing, and sharing scientific workflows. Computational Materials Science, 2021, 188, 110165.	1.4	40
135	NMR shifts for polycyclic aromatic hydrocarbons from firstâ€principles. International Journal of Quantum Chemistry, 2009, 109, 3336-3342.	1.0	39
136	The frontiers and the challenges. Nature Materials, 2016, 15, 381-382.	13.3	39
137	Self-consistent site-dependent DFT+ <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math> study of stoichiometric and defective <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrMnO</mml:mi><mml:mn>3</mml:mn></mml:msub> Physical Review B, 2010, 82, .	1.1	39
138	Automated high-throughput Wannierisation. Npj Computational Materials, 2020, 6, .	3.5	39
139	First-Principles Photoemission Spectroscopy and Orbital Tomography in Molecules from Koopmans-Compliant Functionals. Physical Review Letters, 2015, 114, 166405.	2.9	38
140	Boltzmann Transport in Nanostructures as a Friction Effect. Nano Letters, 2017, 17, 4675-4682.	4.5	38
141	Energetics and cathode voltages of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Li</mml:mi><mml:mi>M</mml:mi><mml:msub><mml:mi> olivines (<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 177 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:	0.0	38
142	First principles calculation of the energy and structure of two solid surface phases on Ir{100}. Surface Science, 1998, 418, 529-535.	0.8	36
143	Transport properties of room-temperature ionic liquids from classical molecular dynamics. Journal of Chemical Physics, 2012, 137, 044508.	1.2	36
144	Donor and acceptor levels of organic photovoltaic compounds from first principles. Physical Chemistry Chemical Physics, 2013, 15, 685-695.	1.3	36

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145	Generalization of Fourierâ€™s Law into Viscous Heat Equations. Physical Review X, 2020, 10, .	2.8	36
146	A Classical and Ab Initio Study of the Interaction of the Myosin Triphosphate Binding Domain with ATP. Biophysical Journal, 2002, 82, 660-675.	0.2	35
147	HP â€“ A code for the calculation of Hubbard parameters using density-functional perturbation theory. Computer Physics Communications, 2022, 279, 108455.	3.0	35
148	Dominant phonon wave vectors and strain-induced splitting of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>2</mml:mn><mml:mi>D</mml:mi></mml:mrow></mml:math>Raman mode of graphene. Physical Review B, 2012, 85, .	1.1	34
149	Koopmans-Compliant Spectral Functionals for Extended Systems. Physical Review X, 2018, 8, .	2.8	34
150	Unique Carbon-Nanotube Field-Effect Transistors with Asymmetric Source and Drain Contacts. Nano Letters, 2008, 8, 64-68.	4.5	33
151	Spin-resolved optical conductivity of two-dimensional group-VIB transition-metal dichalcogenides. Physical Review B, 2014, 90, .	1.1	33
152	Modeling lithium-ion solid-state electrolytes with a pinball model. Physical Review Materials, 2018, 2, .	0.9	33
153	Photoelectron properties of DNA and RNA bases from many-body perturbation theory. Physical Review B, 2011, 84, .	1.1	32
154	Bridging density-functional and many-body perturbation theory: Orbital-density dependence in electronic-structure functionals. Physical Review B, 2014, 89, .	1.1	32
155	Prediction of Phonon-Mediated Superconductivity with High Critical Temperature in the Two-Dimensional Topological Semimetal W₂N₃. Nano Letters, 2021, 21, 3435-3442.	4.5	31
156	Maximally localized Wannier functions in antiferromagnetic MnO within the FLAPW formalism. Physical Review B, 2002, 65, .	1.1	30
157	Dynamical Structure, Bonding, and Thermodynamics of the Superionic Sublattice inÎ±â^’AgI. Physical Review Letters, 2006, 97, 166401.	2.9	30
158	Theoretical Prediction of Two-Dimensional Materials, Behavior, and Properties. ACS Nano, 2021, 15, 5959-5976.	7.3	30
159	Thermodynamic stability of alkali-metalâ€“zinc double-cation borohydrides at low temperatures. Physical Review B, 2013, 88, .	1.1	29
160	Variational minimization of orbital-density-dependent functionals. Physical Review B, 2015, 91, .	1.1	29
161	Nanoscale surface dynamics of Bi₂Te₃(111): observation of a prominent surface acoustic wave and the role of van der Waals interactions. Nanoscale, 2018, 10, 14627-14636.	2.8	27
162	Automated quantum conductance calculations using maximally-localised Wannier functions. Computer Physics Communications, 2011, 182, 2174-2183.	3.0	26

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163	Lattice anharmonicity in lowâ€dimensional carbon systems. Physica Status Solidi (B): Basic Research, 2008, 245, 2149-2154.	0.7	25
164	Ab initioconverse NMR approach for pseudopotentials. Physical Review B, 2010, 81, .	1.1	25
165	Conductance Switching and Many-Valued Logic in Porphyrin Assemblies. Journal of Physical Chemistry Letters, 2013, 4, 3039-3044.	2.1	25
166	Koopmans-Compliant Functionals and Potentials and Their Application to the GW100 Test Set. Journal of Chemical Theory and Computation, 2019, 15, 1905-1914.	2.3	25
167	Dielectric Response of Periodic Systems from Quantum Monte Carlo Calculations. Physical Review Letters, 2005, 95, 207602.	2.9	24
168	Realistic Modeling of Nanostructures Using Density Functional Theory. MRS Bulletin, 2006, 31, 681-687.	1.7	24
169	Carbeneâ€Functionalized Singleâ€Walled Carbon Nanotubes and Their Electrical Properties. Small, 2011, 7, 1257-1263.	5.2	24
170	Electronic, vibrational, and transport properties of pnictogen-substituted ternary skutterudites. Physical Review B, 2012, 85, .	1.1	24
171	A posteriori metadata from automated provenance tracking: integration of AiiDA and TCOD. Journal of Cheminformatics, 2017, 9, 56.	2.8	24
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