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	Nanoscale-Resolved Surface-to-Bulk Electron Transport in CsPbBr₃ Perovskite. Nano Letters, 2022, 22, 1067-1074.	4.5	6
2	Structure Evolution of Graphitic Surface upon Oxidation: Insights by Scanning Tunneling Microscopy. Jacs Au, 2022, 2, 723-730.	3.6	14
3	Unified Green's function approach for spectral and thermodynamic properties from algorithmic inversion of dynamical potentials. Physical Review Research, 2022, 4, .	1.3	2
4	Complex magnetic structure and spin waves of the noncollinear antiferromagnet <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Mn</mml:mi></mml:mrow><mml:mn>5</m Physical Review B, 2022, 105, .	1.1	1
5	Microscopic picture of paraelectric perovskites from structural prototypes. Physical Review Research, 2022, 4, .	1.3	11
6	Energy Level Alignment at the Cobalt Phosphate/Electrolyte Interface: Intrinsic Stability vs Interfacial Chemical Reactions in 5 V Lithium Ion Batteries. ACS Applied Materials & Interfaces, 2022, 14, 543-556.	4.0	4
7	Phonon-Assisted Luminescence in Defect Centers from Many-Body Perturbation Theory. Physical Review Letters, 2022, 128, 167401.	2.9	13
8	HP â€“ A code for the calculation of Hubbard parameters using density-functional perturbation theory. Computer Physics Communications, 2022, 279, 108455.	3.0	35
9	Bloch's theorem in orbital-density-dependent functionals: Band structures from Koopmans spectral functionals. Physical Review B, 2022, 106, .	1.1	5
10	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
11	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
12	AiiDAlab â€“ an ecosystem for developing, executing, and sharing scientific workflows. Computational Materials Science, 2021, 188, 110165.	1.4	40
13	High Li-ion conductivity in tetragonal LGPO: A comparative first-principles study against known LISICON and LGPS phases. Physical Review Materials, 2021, 5, .	0.9	8
14	On the design of solid-state Li-ion batteries. Nature Computational Science, 2021, 1, 179-180.	3.8	1
15	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
16	Theoretical Prediction of Two-Dimensional Materials, Behavior, and Properties. ACS Nano, 2021, 15, 5959-5976.	7.3	30
17	Electronic-structure methods for materials design. Nature Materials, 2021, 20, 736-749.	13.3	96
18	Electronic Structure of Water from Koopmans-Compliant Functionals. Journal of Chemical Theory and Computation, 2021, 17, 3923-3930.	2.3	6

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19	OPTIMADE, an API for exchanging materials data. Scientific Data, 2021, 8, 217.	2.4	49
20	Shear and Breathing Modes of Layered Materials. ACS Nano, 2021, 15, 12509-12534.	7.3	22
21	Gas Transport across Carbon Nitride Nanopores: A Comparison of van der Waals Functionals against the Random-Phase Approximation. Journal of Physical Chemistry C, 2021, 125, 18896-18904.	1.5	4
22	Common workflows for computing material properties using different quantum engines. Npj Computational Materials, 2021, 7, .	3.5	10
23	Gate Control of Spin-Layer-Locking FETs and Application to Monolayer LuIO. Nano Letters, 2021, 21, 7631-7636.	4.5	2
24	Data Management Plans: the Importance of Data Management in the BIGâ€MAP Project**. Batteries and Supercaps, 2021, 4, 1803-1812.	2.4	19
25	Virtual Computational Chemistry Teaching Laboratoriesâ€”Hands-On at a Distance. Journal of Chemical Education, 2021, 98, 3163-3171.	1.1	15
26	AbÂInitio Electron-Phonon Interactions in Correlated Electron Systems. Physical Review Letters, 2021, 127, 126404.	2.9	22
27	Importance of intersite Hubbard interactions in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mml:mrow><mml:mi>Cl</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math> : A first-principles <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:mrow></mml:math> study. Physical Review Materials, 2021, 5, .	0.9	12
28	First-principles predictions of Hall and drift mobilities in semiconductors. Physical Review Research, 2021, 3, .	1.3	48
29	Thermomechanical properties of honeycomb lattices from internal-coordinates potentials: the case of graphene and hexagonal boron nitride. 2D Materials, 2021, 8, 015026.	2.0	7
30	Wannier90 as a community code: new features and applications. Journal of Physics Condensed Matter, 2020, 32, 165902.	0.7	807
31	High-throughput computational screening for solid-state Li-ion conductors. Energy and Environmental Science, 2020, 13, 928-948.	15.6	80
32	Role of OH Intermediates during the Au Oxide Electro-Reduction at Low pH Elucidated by Electrochemical Surface-Enhanced Raman Spectroscopy and Implicit Solvent Density Functional Theory. ACS Catalysis, 2020, 10, 12716-12726.	5.5	17
33	Automated high-throughput Wannierisation. Npj Computational Materials, 2020, 6, .	3.5	39
34	Efficient Kr/Xe separation from triangular g-C₃N₄ nanopores, a simulation study. Journal of Materials Chemistry A, 2020, 8, 17747-17755.	5.2	6
35	Electrosorption at metal surfaces from first principles. Npj Computational Materials, 2020, 6, .	3.5	49
36	AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance. Scientific Data, 2020, 7, 300.	2.4	142

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37	Materials Cloud, a platform for open computational science. Scientific Data, 2020, 7, 299.	2.4	189
38	Li4â€“xGe1â€“xPxO4, a Potential Solid-State Electrolyte for All-Oxide Microbatteries. ACS Applied Energy Materials, 2020, 3, 9910-9917.	2.5	11
39	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> Physical Review Letters, 2020, 124, 206402.	2.9	74
40	The solid-state Li-ion conductor Li7TaO6: A combined computational and experimental study. Solid State Ionics, 2020, 347, 115226.	1.3	6
41	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
42	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
43	Hubbard-corrected density functional perturbation theory with ultrasoft pseudopotentials. Physical Review B, 2020, 101, .	1.1	43
44	Production and processing of graphene and related materials. 2D Materials, 2020, 7, 022001.	2.0	333
45	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
46	Generalization of Fourierâ€™s Law into Viscous Heat Equations. Physical Review X, 2020, 10, .	2.8	36
47	Intrinsic edge excitons in two-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn> Physical Review B, 2020, 101, .	1.1	6
48	Q<scp>uantum</scp> ESPRESSO toward the exascale. Journal of Chemical Physics, 2020, 152, 154105.	1.2	796
49	Operando XANES from first-principles and its application to iridium oxide. Physical Chemistry Chemical Physics, 2020, 22, 10807-10818.	1.3	16
50	Pulay forces in density-functional theory with extended Hubbard functionals: From nonorthogonalized to orthogonalized manifolds. Physical Review B, 2020, 102, .	1.1	22
51	Emergent dual topology in the three-dimensional Kane-Mele Pt2HgSe3. Physical Review Research, 2020, 2, .	1.3	19
52	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> 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> Physical Review Research, 2020, 2, .	1.3	50
53	Electronic structure of pristine and Ni-substituted <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>La</mml:mi><mml:mi>Fe</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow> from near edge x-ray absorption fine structure experiments and first-principles simulations. Physical Review Research, 2020, 2, .	1.3	17
54	On the Kinetic Theory of Thermal Transport in Crystals. , 2020, , 767-808.		0

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55	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	1.3	236
56	Enhanced Electron-Phonon Interaction in Multivalley Materials. Physical Review X, 2019, 9, .	2.8	47
57	Functional Extrapolations to Tame Unbound Anions in Density-Functional Theory Calculations. Journal of Chemical Theory and Computation, 2019, 15, 6313-6322.	2.3	7
58	Absolute band alignment at semiconductor-water interfaces using explicit and implicit descriptions for liquid water. Npj Computational Materials, 2019, 5, .	3.5	48
59	Relative Abundance of Z2 Topological Order in Exfoliable Two-Dimensional Insulators. Nano Letters, 2019, 19, 8431-8440.	4.5	50
60	Yttrium Tantalum Oxynitride Multiphases as Photoanodes for Water Oxidation. Journal of Physical Chemistry C, 2019, 123, 26211-26217.	1.5	9
61	Solvent-Aware Interfaces in Continuum Solvation. Journal of Chemical Theory and Computation, 2019, 15, 1996-2009.	2.3	43
62	Grand canonical simulations of electrochemical interfaces in implicit solvation models. Journal of Chemical Physics, 2019, 150, 041730.	1.2	122
63	Unified theory of thermal transport in crystals and glasses. Nature Physics, 2019, 15, 809-813.	6.5	255
64	Equipartition of Energy Defines the Sizeâ€“Thickness Relationship in Liquid-Exfoliated Nanosheets. ACS Nano, 2019, 13, 7050-7061.	7.3	123
65	Valley-Engineering Mobilities in Two-Dimensional Materials. Nano Letters, 2019, 19, 3723-3729.	4.5	23
66	Koopmans Meets Betheâ€“Salpeter: Excitonic Optical Spectra without GW. Journal of Chemical Theory and Computation, 2019, 15, 3710-3720.	2.3	20
67	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></mml:math> Physical Review B, 2019, 99, .	1.1	39
68	SIMPLE code: Optical properties with optimal basis functions. Computer Physics Communications, 2019, 240, 106-119.	3.0	21
69	Photorealistic modelling of metals from first principles. Npj Computational Materials, 2019, 5, .	3.5	21
70	Halogen-bond driven self-assembly of perfluorocarbon monolayers on silicon nitride. Journal of Materials Chemistry A, 2019, 7, 24445-24453.	5.2	10
71	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
72	Continuum models of the electrochemical diffuse layer in electronic-structure calculations. Journal of Chemical Physics, 2019, 150, 041722.	1.2	57

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73	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
74	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 ETQq0 0 0 rgBT /Overlock 10 Tf 50 697 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow	3.9	38
75	Unsupervised landmark analysis for jump detection in molecular dynamics simulations. Physical Review Materials, 2019, 3, .	0.9	24
76	Screening in Orbital-Density-Dependent Functionals. Journal of Chemical Theory and Computation, 2018, 14, 2549-2557.	2.3	13
77	Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. Nature Nanotechnology, 2018, 13, 246-252.	15.6	1,317
78	Prediction of a Large-Gap and Switchable Kane-Mele Quantum Spin Hall Insulator. Physical Review Letters, 2018, 120, 117701.	2.9	79
79	Precision and efficiency in solid-state pseudopotential calculations. Npj Computational Materials, 2018, 4, .	3.5	390
80	Screw dislocation structure and mobility in body centered cubic Fe predicted by a Gaussian Approximation Potential. Npj Computational Materials, 2018, 4, .	3.5	63
81	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
82	On the Kinetic Theory of Thermal Transport in Crystals. , 2018, , 1-42.		0
83	Koopmans-Compliant Spectral Functionals for Extended Systems. Physical Review X, 2018, 8, .	2.8	34
84	Vibrational and thermoelastic properties of bcc iron from selected EAM potentials. Computational Materials Science, 2018, 152, 99-106.	1.4	8
85	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
86	Hubbard parameters from density-functional perturbation theory. Physical Review B, 2018, 98, .	1.1	194
87	Novel 2-D Materials for Tunneling FETs: an Ab-initio Study. , 2018, , .		0
88	Potential-induced nanoclustering of metallic catalysts during electrochemical CO2 reduction. Nature Communications, 2018, 9, 3117.	5.8	253
89	<italic>Ab Initio</italic> Simulation of Band-to-Band Tunneling FETs With Single- and Few-Layer 2-D Materials as Channels. IEEE Transactions on Electron Devices, 2018, 65, 4180-4187.	1.6	23
90	Achieving DFT accuracy with a machine-learning interatomic potential: Thermomechanics and defects in bcc ferromagnetic iron. Physical Review Materials, 2018, 2, .	0.9	175

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91	Modeling lithium-ion solid-state electrolytes with a pinball model. Physical Review Materials, 2018, 2, .	0.9	33
92	Mobility of two-dimensional materials from first principles in an accurate and automated framework. Physical Review Materials, 2018, 2, .	0.9	93
93	Piezoelectric softening by Nb substitution in (Ba,Pb)ZrO₃ ceramics. Journal of the American Ceramic Society, 2017, 100, 1885-1895.	1.9	3
94	Breakdown of Optical Phononsâ€™ Splitting in Two-Dimensional Materials. Nano Letters, 2017, 17, 3758-3763.	4.5	127
95	Soft-Sphere Continuum Solvation in Electronic-Structure Calculations. Journal of Chemical Theory and Computation, 2017, 13, 3829-3845.	2.3	76
96	Highly Active and Stable Iridium Pyrochlores for Oxygen Evolution Reaction. Chemistry of Materials, 2017, 29, 5182-5191.	3.2	172
97	Determination of Conduction and Valence Band Electronic Structure of LaTiO x N y Thin Film. ChemSusChem, 2017, 10, 2099-2106.	3.6	19
98	Unraveling Thermodynamics, Stability, and Oxygen Evolution Activity of Strontium Ruthenium Perovskite Oxide. ACS Catalysis, 2017, 7, 3245-3256.	5.5	113
99	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	0.7	4,303
100	Boltzmann Transport in Nanostructures as a Friction Effect. Nano Letters, 2017, 17, 4675-4682.	4.5	38
101	Enhanced Proton Conductivity in Yâ€Doped BaZrO₃ via Strain Engineering. Advanced Science, 2017, 4, 1700467.	5.6	45
102	A posteriori metadata from automated provenance tracking: integration of AiiDA and TCOD. Journal of Cheminformatics, 2017, 9, 56.	2.8	24
103	Ionic correlations and failure of Nernst-Einstein relation in solid-state electrolytes. Physical Review Materials, 2017, 1, .	0.9	86
104	Transport waves as crystal excitations. Physical Review Materials, 2017, 1, .	0.9	20
105	A generalized Poisson and Poisson-Boltzmann solver for electrostatic environments. Journal of Chemical Physics, 2016, 144, 014103.	1.2	88
106	First-principles molecular dynamics simulations of proton diffusion in cubic BaZrO $$_3$$ 3 perovskite under strain conditions. Materials for Renewable and Sustainable Energy, 2016, 5, 1.	1.5	12
107	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
108	Asymmetric structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mn>90</mml:mn><mml:mo>â~</mml:mo></mml:msup></m walls and interactions with defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>PbTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review B, 2016, 93, .	1.1	22

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109	Thermal Transport in Crystals as a Kinetic Theory of Relaxons. Physical Review X, 2016, 6, .	2.8	72
110	Performance of arsenene and antimonene double-gate MOSFETs from first principles. Nature Communications, 2016, 7, 12585.	5.8	278
111	First-Principles Photoemission Spectroscopy of DNA and RNA Nucleobases from Koopmans-Compliant Functionals. Journal of Chemical Theory and Computation, 2016, 12, 3948-3958.	2.3	12
112	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
113	The frontiers and the challenges. Nature Materials, 2016, 15, 381-382.	13.3	39
114	The Electronic Thermal Conductivity of Graphene. Nano Letters, 2016, 16, 2439-2443.	4.5	137
115	AiiDA: automated interactive infrastructure and database for computational science. Computational Materials Science, 2016, 111, 218-230.	1.4	399
116	Integration of Theoretical Crystallography Open Database and AiiDA. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s494-s494.	0.0	0
117	Phonon hydrodynamics in two-dimensional materials. Nature Communications, 2015, 6, 6400.	5.8	385
118	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
119	Bandâ€Like Electron Transport with Recordâ€High Mobility in the TCNQ Family. Advanced Materials, 2015, 27, 2453-2458.	11.1	122
120	Self-consistent continuum solvation for optical absorption of complex molecular systems in solution. Journal of Chemical Physics, 2015, 142, 034111.	1.2	17
121	First-principles investigation of organic photovoltaic materials<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>C</mml:mtext><mml:mn>60</mml:mn></mml:msub> and bis-<mml:math xmlns:mml="h. Physical Review B, 2015, 91, .	11	21
122	Variational minimization of orbital-density-dependent functionals. Physical Review B, 2015, 91, .	1.1	29
123	First-Principles Photoemission Spectroscopy and Orbital Tomography in Molecules from Koopmans-Compliant Functionals. Physical Review Letters, 2015, 114, 166405.	2.9	38
124	Large-Area Epitaxial Monolayer MoS₂. ACS Nano, 2015, 9, 4611-4620.	7.3	712
125	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
126	Emergence of One-Dimensional Wires of Free Carriers in Transition-Metal-Dichalcogenide Nanostructures. Nano Letters, 2015, 15, 6229-6238.	4.5	85

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127	Spin-resolved optical conductivity of two-dimensional group-VIB transition-metal dichalcogenides. Physical Review B, 2014, 90, .	1.1	33
128	Koopmans-compliant functionals and their performance against reference molecular data. Physical Review B, 2014, 90, .	1.1	81
129	Static Dielectric Permittivity of Ice from First Principles. Physical Review Letters, 2014, 113, 245501.	2.9	7
130	An updated version of wannier90: A tool for obtaining maximally-localised Wannier functions. Computer Physics Communications, 2014, 185, 2309-2310.	3.0	1,561
131	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
132	Piecewise Linearity and Spectroscopic Properties from Koopmans-Compliant Functionals. Topics in Current Chemistry, 2014, 347, 193-233.	4.0	19
133	Thermal Conductivity of Graphene and Graphite: Collective Excitations and Mean Free Paths. Nano Letters, 2014, 14, 6109-6114.	4.5	449
134	An Open-Source Multiscale Framework for the Simulation of Nanoscale Devices. IEEE Transactions on Electron Devices, 2014, 61, 48-53.	1.6	56
135	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
136	Bridging density-functional and many-body perturbation theory: Orbital-density dependence in electronic-structure functionals. Physical Review B, 2014, 89, .	1.1	32
137	Engineering polar discontinuities in honeycomb lattices. Nature Communications, 2014, 5, 5157.	5.8	43
138	Electronâ€“Phonon Interactions and the Intrinsic Electrical Resistivity of Graphene. Nano Letters, 2014, 14, 1113-1119.	4.5	149
139	An updated version of BoltzWann: A code for the evaluation of thermoelectric and electronic transport properties with a maximally-localized Wannier functions basis. Computer Physics Communications, 2014, 185, 2311-2312.	3.0	10
140	Chemisorbed Molecules under Potential Bias: Detailed Insights from First-Principles Vibrational Spectroscopies. Electrochimica Acta, 2014, 121, 210-214.	2.6	22
141	Electrostatics of solvated systems in periodic boundary conditions. Physical Review B, 2014, 90, .	1.1	71
142	First-Principles Determination of Phonon Lifetimes, Mean Free Paths, and Thermal Conductivities in Crystalline Materials: Pure Silicon and Germanium. Topics in Applied Physics, 2014, , 115-136.	0.4	9
143	Covalently Functionalized Metallic Single-Walled Carbon Nanotubes Studied Using Electrostatic Force Microscopy and Dielectric Force Microscopy. Journal of Physical Chemistry C, 2013, 117, 24570-24578.	1.5	11
144	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

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145	Conductance Switching and Many-Valued Logic in Porphyrin Assemblies. Journal of Physical Chemistry Letters, 2013, 4, 3039-3044.	2.1	25
146	Donor and acceptor levels of organic photovoltaic compounds from first principles. Physical Chemistry Chemical Physics, 2013, 15, 685-695.	1.3	36
147	Self-assembled quantum dots in a nanowire system for quantum photonics. Nature Materials, 2013, 12, 439-444.	13.3	306
148	First-Principles Prediction of the Equilibrium Shape of Nanoparticles Under Realistic Electrochemical Conditions. Physical Review Letters, 2013, 110, 086104.	2.9	57
149	Quantum states of muons in fluorides. Physical Review B, 2013, 87, .	1.1	57
150	First-principles quantum transport with electron-vibration interactions: A maximally localized Wannier functions approach. Physical Review B, 2013, 87, .	1.1	15
151	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
152	A Natural Helical Crystal Lattice Model for Carbon Nanotubes. Journal of Chemical Theory and Computation, 2013, 9, 1865-1871.	2.3	5
153	Thermodynamic stability of alkali-metalâ€“zinc double-cation borohydrides at low temperatures. Physical Review B, 2013, 88, .	1.1	29
154	Correction for Centrone et al., 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, 2013, 110, 6241-6241.	3.3	3
155	Self-consistent continuum solvation (SCCS): The case of charged systems. Journal of Chemical Physics, 2013, 139, 214110.	1.2	90
156	Playing quantum hide-and-seek with the muon: localizing muon stopping sites. Physica Scripta, 2013, 88, 068510.	1.2	67
157	An integrated framework for multi-scale multi-physics numerical modelling of interface evolution in welding. IOP Conference Series: Materials Science and Engineering, 2012, 33, 012029.	0.3	5
158	Transport properties of room-temperature ionic liquids from classical molecular dynamics. Journal of Chemical Physics, 2012, 137, 044508.	1.2	36
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