Miguel A L Marques

List of Publications by Year
in descending order

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190 papers	14,393 citations	31974 53 h-index	20955 115 g-index
199 all docs	199 docs citations	199 times ranked	12287 citing authors

#	Article	IF	Citations
1	Recent advances and applications of machine learning in solid-state materials science. Npj Computational Materials, 2019, 5, .	8.7	1,289
2	TIME-DEPENDENT DENSITY FUNCTIONAL THEORY. Annual Review of Physical Chemistry, 2004, 55, 427-455.	10.8	1,099
3	octopus: a tool for the application of time-dependent density functional theory. Physica Status Solidi (B): Basic Research, 2006, 243, 2465-2488.	1.5	756
4	octopus: a first-principles tool for excited electronâ€“ion dynamics. Computer Physics Communications, 2003, 151, 60-78.	7.5	671
5	Propagators for the time-dependent Kohnâ€“Sham equations. Journal of Chemical Physics, 2004, 121, 3425-3433.	3.0	477
6	Libxc: A library of exchange and correlation functionals for density functional theory. Computer Physics Communications, 2012, 183, 2272-2281.	7.5	419
7	Real-space grids and the Octopus code as tools for the development of new simulation approaches for electronic systems. Physical Chemistry Chemical Physics, 2015, 17, 31371-31396.	2.8	376
8	The Abinitproject: Impact, environment and recent developments. Computer Physics Communications, 2020, 248, 107042.	7.5	369
9	Recent developments in libxc â€” A comprehensive library of functionals for density functional theory. SoftwareX, 2018, 7, 1-5.	2.6	367
10	Density-based mixing parameter for hybrid functionals. Physical Review B, 2011, 83, .	3.2	338
11	Ab initiotheory of superconductivity. I. Density functional formalism and approximate functionals. Physical Review B, 2005, 72, .	3.2	314
12	Crystal Structure of Cold Compressed Graphite. Physical Review Letters, 2012, 108, 065501.	7.8	292
13	Ab initiotheory of superconductivity. II. Application to elemental metals. Physical Review B, 2005, 72, .	3.2	261
14	Stability and electronic properties of new inorganic perovskites from high-throughput ab initio calculations. Journal of Materials Chemistry C, 2016, 4, 3157-3167.	5.5	235
15	Predicting the Thermodynamic Stability of Solids Combining Density Functional Theory and Machine Learning. Chemistry of Materials, 2017, 29, 5090-5103.	6.7	217
16	Octopus, a computational framework for exploring light-driven phenomena and quantum dynamics in extended and finite systems. Journal of Chemical Physics, 2020, 152, 124119.	3.0	210
17	Benchmarking the Starting Points of the GW Approximation for Molecules. Journal of Chemical Theory and Computation, 2013, 9, 324-329.	5.3	206
18	Time-Dependent Density-Functional Approach for Biological Chromophores: The Case of the Green Fluorescent Protein. Physical Review Letters, 2003, 90, 258101.	7.8	181

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19	Time-dependent density-functional theory in massively parallel computer architectures: the octopus project. Journal of Physics Condensed Matter, 2012, 24, 233202.	1.8	181
20	Superconductivity in Lithium, Potassium, and Aluminum under Extreme Pressure: A First-Principles Study. Physical Review Letters, 2006, 96, 047003.	7.8	159
21	Exchange-correlation functionals for band gaps of solids: benchmark, reparametrization and machine learning. Npj Computational Materials, 2020, 6, .	8.7	156
22	Large-Scale Benchmark of Exchangeâ€“Correlation Functionals for the Determination of Electronic Band Gaps of Solids. Journal of Chemical Theory and Computation, 2019, 15, 5069-5079.	5.3	151
23	Direct Observation of the Mechanical Properties of Single-Walled Carbon Nanotubes and Their Junctions at the Atomic Level. Nano Letters, 2003, 3, 751-755.	9.1	148
24	Low-energy silicon allotropes with strong absorption in the visible for photovoltaic applications. Physical Review B, 2012, 86, .	3.2	138
25	Accuracy of generalized gradient approximation functionals for density-functional perturbation theory calculations. Physical Review B, 2014, 89, .	3.2	138
26	Superconducting Properties ofMgB2from First Principles. Physical Review Letters, 2005, 94, 037004.	7.8	137
27	Excited states dynamics in time-dependent density functional theory. European Physical Journal D, 2004, 28, 211-218.	1.3	126
28	Time-dependent electron localization function. Physical Review A, 2005, 71, .	2.5	122
29	A TDDFT Study of the Excited States of DNA Bases and Their Assemblies. Journal of Physical Chemistry B, 2006, 110, 7129-7138.	2.6	112
30	Band structures of Cu2ZnSnS4 and Cu2ZnSnSe4 from many-body methods. Applied Physics Letters, 2011, 98, 241915.	3.3	112
31	Time-dependent density functional theory scheme for efficient calculations of dynamic (hyper)polarizabilities. Journal of Chemical Physics, 2007, 126, 184106.	3.0	106
32	Prediction of Stable Nitride Perovskites. Chemistry of Materials, 2015, 27, 5957-5963.	6.7	102
33	Probing Time-Dependent Molecular Dipoles on the Attosecond Time Scale. Physical Review Letters, 2013, 111, 033001.	7.8	99
34	Benchmark Many-Body GW and Betheâ€“Salpeter Calculations for Small Transition Metal Molecules. Journal of Chemical Theory and Computation, 2014, 10, 3934-3943.	5.3	98
35	On the Breaking of Carbon Nanotubes under Tension. Nano Letters, 2004, 4, 811-815.	9.1	91
36	Density-matrix-power functional: Performance for finite systems and the homogeneous electron gas. Physical Review A, 2009, 79, .	2.5	91

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37	Effects of Electronic and Lattice Polarization on the Band Structure of Delafossite Transparent Conductive Oxides. Physical Review Letters, 2010, 104, 136401.	7.8	88
38	High-Pressure Structures of Disilane and Their Superconducting Properties. Physical Review Letters, 2012, 108, 117004.	7.8	86
39	Ab initioangle- and energy-resolved photoelectron spectroscopy with time-dependent density-functional theory. Physical Review A, 2012, 85, .	2.5	82
40	Empirical functionals for reduced-density-matrix-functional theory. Physical Review A, 2008, 77, .	2.5	77
41	Benchmark calculations for reduced density-matrix functional theory. Journal of Chemical Physics, 2008, 128, 184103.	3.0	70
42	Low-density silicon allotropes for photovoltaic applications. Physical Review B, 2015, 92, .	3.2	70
43	Optical Absorption of the Blue Fluorescent Protein: A First-Principles Study. Journal of the American Chemical Society, 2005, 127, 12329-12337.	13.7	69
44	Magnetic response and NMR spectra of carbon nanotubes fromab initiocalculations. Physical Review B, 2006, 73, .	3.2	69
45	Propagators for the Time-Dependent Kohnâ€“Sham Equations: Multistep, Rungeâ€“Kutta, Exponential Rungeâ€“Kutta, and Commutator Free Magnus Methods. Journal of Chemical Theory and Computation, 2018, 14, 3040-3052.	5.3	69
46	Roadmap on Machine learning in electronic structure. Electronic Structure, 2022, 4, 023004.	2.8	69
47	Time-Dependent Density Functional Theory. Lecture Notes in Physics, 2003, , 144-184.	0.7	63
48	Band structures of delafossite transparent conductive oxides from a self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>approach. Physical Review B, 2010, 82, .	3.2	63
49	Machine Learning the Physical Nonlocal Exchangeâ€“Correlation Functional of Density-Functional Theory. Journal of Physical Chemistry Letters, 2019, 10, 6425-6431.	4.6	62
50	Density functional theory beyond the linear regime: Validating an adiabatic local density approximation. Physical Review A, 2011, 83, .	2.5	61
51	Sodiumâ€“gold binaries: novel structures for ionic compounds from anab initiostructural search. New Journal of Physics, 2013, 15, 115007.	2.9	58
52	Strong Renormalization of the Electronic Band Gap due to Lattice Polarization in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:math>Formalism. Physical Review Letters, 2013, 110, 226404.	7.8	56
53	Identification of Novel Cu, Ag, and Au Ternary Oxides from Global Structural Prediction. Chemistry of Materials, 2015, 27, 4562-4573.	6.7	56
54	Can optical spectroscopy directly elucidate the ground state of C20?. Journal of Chemical Physics, 2002, 116, 1930-1933.	3.0	55

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55	First-Principles Identification of Single Photon Emitters Based on Carbon Clusters in Hexagonal Boron Nitride. Journal of Physical Chemistry A, 2021, 125, 1325-1335.	2.5	51
56	Optical and magnetic properties of boron fullerenes. Physical Chemistry Chemical Physics, 2009, 11, 4523.	2.8	50
57	The optimal one dimensional periodic table: a modified Pettifor chemical scale from data mining. New Journal of Physics, 2016, 18, 093011.	2.9	50
58	Fragment molecular orbital investigation of the role of AMP protonation in firefly luciferase pH-sensitivity. Physical Chemistry Chemical Physics, 2010, 12, 14285.	2.8	48
59	Identification of fullerene-like CdSe nanoparticles from optical spectroscopy calculations. Physical Review B, 2007, 75, .	3.2	47
60	The planar-to-tubular structural transition in boron clusters from optical absorption. Journal of Chemical Physics, 2005, 123, 014310.	3.0	46
61	Superconducting properties of MgB2 from first principles. Physica C: Superconductivity and Its Applications, 2007, 456, 45-53.	1.2	46
62	Towards a gauge invariant method for molecular chiroptical properties in TDDFT. Physical Chemistry Chemical Physics, 2009, 11, 4481.	2.8	46
63	Insights into colour-tuning of chlorophyll optical response in green plants. Physical Chemistry Chemical Physics, 2015, 17, 26599-26606.	2.8	46
64	High-throughput search of ternary chalcogenides for p-type transparent electrodes. Scientific Reports, 2017, 7, 43179.	3.3	46
65	Advanced Raman spectroscopy of Cs2AgBiBr6 double perovskites and identification of Cs3Bi2Br9 secondary phases. Scripta Materialia, 2020, 184, 24-29.	5.2	46
66	Towards a formal definition of static and dynamic electronic correlations. Physical Chemistry Chemical Physics, 2017, 19, 12655-12664.	2.8	44
67	Novel Structural Motifs in Low Energy Phases of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>LiAlH</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 108, 205505.	7.8	43
68	Speeding up the solution of the Bethe-Salpeter equation by a double-grid method and Wannier interpolation. Physical Review B, 2012, 86, .	3.2	42
69	Local Modified Becke-Johnson Exchange-Correlation Potential for Interfaces, Surfaces, and Two-Dimensional Materials. Journal of Chemical Theory and Computation, 2020, 16, 2654-2660.	5.3	42
70	An Application of Non-Extensive Statistical Mechanics to Nanosystems. Journal of Computational and Theoretical Nanoscience, 2004, 1, 227-229.	0.4	42
71	Ab initioprediction of pressure-induced superconductivity in potassium. Physical Review B, 2006, 73, .	3.2	41
72	From mesoscale to nanoscale mechanics in single-wall carbon nanotubes. Carbon, 2017, 123, 145-150.	10.3	41

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73	Semilocal exchange-correlation potentials for solid-state calculations: Current status and future directions. Journal of Applied Physics, 2019, 126, .	2.5	41
74	Predicting stable crystalline compounds using chemical similarity. Npj Computational Materials, 2021, 7, .	8.7	41
75	A Tutorial on Density Functional Theory. Lecture Notes in Physics, 2003, , 218-256.	0.7	40
76	Conducting Boron Sheets Formed by the Reconstruction of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-Boron (111) Surface. Physical Review Letters, 2013, 111, 136101.	7.8	40
77	Density-functional tight-binding study of the collapse of carbon nanotubes under hydrostatic pressure. Carbon, 2014, 69, 355-360.	10.3	40
78	Stable hybrid organicâ€“inorganic halide perovskites for photovoltaics from ab initio high-throughput calculations. Journal of Materials Chemistry A, 2018, 6, 6463-6475.	10.3	40
79	Generalized Pauli constraints in reduced density matrix functional theory. Journal of Chemical Physics, 2015, 142, 154108.	3.0	39
80	Low-Energy Polymeric Phases of Alanates. Physical Review Letters, 2013, 110, 135502.	7.8	38
81	Accurate Color Tuning of Firefly Chromophore by Modulation of Local Polarization Electrostatic Fields. Journal of Physical Chemistry B, 2011, 115, 329-332.	2.6	37
82	Crystal graph attention networks for the prediction of stable materials. Science Advances, 2021, 7, eabi7948.	10.3	37
83	The role of dimensionality on the quenching of spin-orbit effects in the optics of gold nanostructures. Journal of Chemical Physics, 2008, 129, 144110.	3.0	36
84	Time-dependent density-functional theory. Physical Chemistry Chemical Physics, 2009, 11, 4436.	2.8	34
85	Computational acceleration of prospective dopant discovery in cuprous iodide. Physical Chemistry Chemical Physics, 2019, 21, 18839-18849.	2.8	34
86	Mechanism of surface passivation of methylammonium lead tribromide single crystals by benzylamine. Applied Physics Reviews, 2019, 6, 031401.	11.3	34
87	Carbon structures and defect planes in diamond at high pressure. Physical Review B, 2013, 88, .	3.2	32
88	Double perovskites as p-type conducting transparent semiconductors: a high-throughput search. Journal of Materials Chemistry A, 2019, 7, 14705-14711.	10.3	32
89	Efficient calculation of van der Waals dispersion coefficients with time-dependent density functional theory in real time: Application to polycyclic aromatic hydrocarbons. Journal of Chemical Physics, 2007, 127, 014107.	3.0	31
90	Predicting the stability of ternary intermetallics with density functional theory and machine learning. Journal of Chemical Physics, 2018, 148, 241728.	3.0	30

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91	Bioheterojunction Effect on Fluorescence Origin and Efficiency Improvement of Firefly Chromophores. Journal of Physical Chemistry Letters, 2010, 1, 2781-2787.	4.6	29
92	Density gradients for the exchange energy of electrons in two dimensions. Physical Review A, 2009, 79, .	2.5	28
93	Raman activity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>s</mml:mi><mml:msup><mml:mi>p</mml:mi><mml:mn>3</mml:mn></mml:msup></mml:m allotropes under pressure: A density functional theory study. Physical Review B, 2012, 85, .	3.2	28
94	Radial collapse of carbon nanotubes for conductivity optimized polymer composites. Carbon, 2016, 106, 64-73.	10.3	28
95	Pressure-induced radial collapse in few-wall carbon nanotubes: A combined theoretical and experimental study. Carbon, 2017, 125, 429-436.	10.3	27
96	Cluster-surface and cluster-cluster interactions:Ab initiocalculations and modeling of asymptotic van der Waals forces. Physical Review B, 2008, 78, .	3.2	26
97	Bandgap of two-dimensional materials: Thorough assessment of modern exchangeâ€“correlation functionals. Journal of Chemical Physics, 2021, 155, 104103.	3.0	26
98	Local correlation functional for electrons in two dimensions. Physical Review B, 2008, 78, .	3.2	25
99	First-principles predicted low-energy structures of NaSc(BH4)4. Journal of Chemical Physics, 2014, 140, 124708.	3.0	25
100	Materials Design On-the-Fly. Journal of Chemical Theory and Computation, 2015, 11, 3955-3960.	5.3	25
101	The ground state of two-dimensional silicon. 2D Materials, 2018, 5, 035010.	4.4	25
102	Neural network force fields for simple metals and semiconductors: construction and application to the calculation of phonons and melting temperatures. Physical Chemistry Chemical Physics, 2019, 21, 6506-6516.	2.8	25
103	Rare-earth magnetic nitride perovskites. JPhys Materials, 2019, 2, 025003.	4.2	25
104	Validation of Pseudopotential Calculations for the Electronic Band Gap of Solids. Journal of Chemical Theory and Computation, 2020, 16, 3620-3627.	5.3	25
105	Excitonic effects in the optical properties of CdSe nanowires. Applied Physics Letters, 2010, 96, .	3.3	24
106	Optical properties of Cu-chalcogenide photovoltaic absorbers from self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:n the Bethe-Salpeter equation. Physical Review B, 2015, 91, .	3.2	24
107	Emergence of superconductivity in doped H2O ice at high pressure. Scientific Reports, 2017, 7, 6825.	3.3	23
108	Reduced Density Matrix Functional Theory for Bosons. Physical Review Letters, 2020, 124, 180603.	7.8	23

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109	The challenge of predicting optical properties of biomolecules: What can we learn from time-dependent density-functional theory?. Comptes Rendus Physique, 2009, 10, 469-490.	0.9	22
110	Superconductivity in layered binary silicides: A density functional theory study. Physical Review B, 2011, 84, .	3.2	21
111	Kirzhnits gradient expansion in two dimensions. Physical Review B, 2012, 85, .	3.2	21
112	Optimized Exchange and Correlation Semilocal Functional for the Calculation of Energies of Formation. Journal of Chemical Theory and Computation, 2015, 11, 3844-3850.	5.3	21
113	Novel crystal structures for lithiumâ€“silicon alloy predicted by minima hopping method. Journal of Alloys and Compounds, 2016, 655, 147-154.	5.5	21
114	Local Hybrid Density Functional for Interfaces. Journal of Chemical Theory and Computation, 2018, 14, 939-947.	5.3	21
115	Accurate electronic band gaps of two-dimensional materials from the local modified Becke-Johnson potential. Physical Review B, 2020, 101, .	3.2	21
116	Optical Properties of Nanostructures from Time-Dependent Density Functional Theory. Journal of Computational and Theoretical Nanoscience, 2004, 1, 231-255.	0.4	21
117	Atomic and electronic properties of quasi-one-dimensional MoS₂ nanowires. Journal of Materials Research, 2013, 28, 240-249.	2.6	20
118	Toward an All-Around Semilocal Potential for Electronic Exchange. Journal of Chemical Theory and Computation, 2010, 6, 3664-3670.	5.3	19
119	Full Color Modulation of Firefly Luciferase through Engineering with Unified Stark Effect. Journal of Physical Chemistry B, 2013, 117, 13725-13730.	2.6	19
120	Structural prediction of two-dimensional materials under strain. 2D Materials, 2017, 4, 045009.	4.4	19
121	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
122	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>Doping in Expanded Phases of ZnO: AnAbÂInitioStudy. Physical Review Letters, 2012, 108, 115903.	7.8	18
123	Efficient Automatized Density-Functional Tight-Binding Parametrizations: Application to Group IV Elements. Journal of Chemical Theory and Computation, 2018, 14, 2947-2954.	5.3	18
124	Reduced density matrix functional theory for superconductors. Physical Review B, 2019, 99, .	3.2	18
125	A high-throughput study of oxynitride, oxyfluoride and nitrofluoride perovskites. Journal of Materials Chemistry A, 2021, 9, 8501-8513.	10.3	18
126	Enhancing the Superconducting Transition Temperature of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BaSi</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>by Structural Tuning. Physical Review Letters, 2011, 106, 087002.	7.8	17

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127	Construction of the B88 Exchange-Energy Functional in Two Dimensions. Journal of Chemical Theory and Computation, 2014, 10, 1837-1842.	5.3	17
128	Relating correlation measures: The importance of the energy gap. Physical Review A, 2017, 95, .	2.5	17
129	Stable Ordered Phases of Cuprous Iodide with Complexes of Copper Vacancies. Chemistry of Materials, 2019, 31, 7877-7882.	6.7	17
130	Nitrogen-hydrogen-oxygen ternary phase diagram: New phases at high pressure from structural prediction. Physical Review Materials, 2018, 2, .	2.4	17
131	On the Use of Neumann's Principle for the Calculation of the Polarizability Tensor of Nanostructures. Journal of Nanoscience and Nanotechnology, 2008, 8, 3392-3398.	0.9	16
132	Nanostructured water and carbon dioxide inside collapsing carbon nanotubes at high pressure. Physical Chemistry Chemical Physics, 2016, 18, 19926-19932.	2.8	16
133	Benchmarking the AK13 Exchange Functional: Ionization Potentials and Electron Affinities. Journal of Chemical Theory and Computation, 2014, 10, 5625-5629.	5.3	15
134	Prediction and Synthesis of a Non-Zintl Silicon Clathrate. Chemistry of Materials, 2016, 28, 3711-3717.	6.7	15
135	Investigation of new phases in the Baâ€“Si phase diagram under high pressure using ab initio structural search. Physical Chemistry Chemical Physics, 2016, 18, 8108-8114.	2.8	15
136	Density functional theory for superconductors. International Journal of Quantum Chemistry, 2004, 99, 790-797.	2.0	14
137	Response Functions in TDDFT: Concepts and Implementation. Lecture Notes in Physics, 2012, , 139-166.	0.7	14
138	Novel phases of lithium-aluminum binaries from first-principles structural search. Journal of Chemical Physics, 2015, 142, 024710.	3.0	14
139	Structural prediction of stabilized atomically thin tin layers. Npj 2D Materials and Applications, 2019, 3, .	7.9	14
140	A viable way to tailor carbon nanomaterials by irradiation-induced transformations. Radiation Physics and Chemistry, 2005, 73, 334-339.	2.8	13
141	Prediction of a novel monoclinic carbon allotrope. European Physical Journal B, 2013, 86, 1.	1.5	13
142	Violation of a local form of the Lieb-Oxford bound. Physical Review A, 2012, 85, .	2.5	12
143	Ab Initio Electronic Gaps of Ge Nanodots: The Role of Self-Energy Effects. Journal of Physical Chemistry C, 2013, 117, 14229-14234.	3.1	12
144	The crystal structure of p-type transparent conductive oxide CuBO2. MRS Communications, 2013, 3, 157-160.	1.8	12

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145	Topological Crystalline Insulator in a New Bi Semiconducting Phase. Scientific Reports, 2016, 6, 21790.	3.3	12
146	On the time evolution of fermionic occupation numbers. Journal of Chemical Physics, 2019, 151, 044112.	3.0	12
147	Time and energy-resolved two photon photoemission of the Cu(100) and Cu(111) metal surfaces. Computational Materials Science, 2004, 30, 110-115.	3.0	11
148	Research Update: Stable single-phase Zn-rich Cu2ZnSnSe4 through In doping. APL Materials, 2016, 4, 070701.	5.1	11
149	Superconductivity in antiperovskites. Npj Computational Materials, 2022, 8, .	8.7	11
150	Superconductivity in an expanded phase of ZnO: anab initiostudy. New Journal of Physics, 2015, 17, 043034.	2.9	10
151	Static correlated functionals for reduced density matrix functional theory. European Physical Journal B, 2018, 91, 1.	1.5	10
152	On the calculation of the bandgap of periodic solids with MGGA functionals using the total energy. Journal of Chemical Physics, 2019, 151, 161102.	3.0	10
153	Direct insight into the structure-property relation of interfaces from constrained crystal structure prediction. Nature Communications, 2021, 12, 811.	12.8	10
154	Electronic Structure of Molecules, Surfaces, and Molecules on Surfaces with the Local Modified Beckeâ€“Johnson Exchangeâ€“Correlation Potential. Journal of Chemical Theory and Computation, 2021, 17, 4746-4755.	5.3	10
155	Machine learning the derivative discontinuity of density-functional theory. Machine Learning: Science and Technology, 2022, 3, 015011.	5.0	10
156	Ab initio calculations of the ground and excited states of the YN molecule including spinâ€“orbit effects. Chemical Physics, 2014, 429, 33-43.	1.9	9
157	High-pressure phases of VO2 from the combination of Raman scattering and ab initio structural search. Physical Review B, 2018, 97, .	3.2	9
158	Novel two-dimensional siliconâ€“carbon binaries by crystal structure prediction. Physical Chemistry Chemical Physics, 2020, 22, 8442-8449.	2.8	8
159	A dataset of 175k stable and metastable materials calculated with the PBEsol and SCAN functionals. Scientific Data, 2022, 9, 64.	5.3	8
160	Specification of an extensible and portable file format for electronic structure and crystallographic data. Computational Materials Science, 2008, 43, 1056-1065.	3.0	7
161	Superior carbon nanotube stability by molecular filling:a single-chirality study at extreme pressures. Carbon, 2021, 183, 884-892.	10.3	7
162	Machine-learning correction to density-functional crystal structure optimization. MRS Bulletin, 2022, 47, 765-771.	3.5	7

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163	Simple preconditioning for time-dependent density functional perturbation theory. Journal of Chemical Physics, 2011, 135, 014103.	3.0	6
164	Optimal control of the electronic current density: Application to one- and two-dimensional one-electron systems. Physical Review A, 2011, 83, .	2.5	6
165	Detection of Cu2Zn5SnSe8 and Cu2Zn6SnSe9 phases in co-evaporated Cu2ZnSnSe4 thin-films. Applied Physics Letters, 2015, 107, .	3.3	6
166	Atomically Thin Pythagorean Tilings in Two Dimensions. Journal of Physical Chemistry Letters, 2021, 12, 4972-4979.	4.6	6
167	Alloying effects on the optical properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ge</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> from time-dependent density functional theory and comparison with effective-medium theory. Physical Review B, 2009, 79, .	3.2	5
168	Modeling van der Waals interactions between proteins and inorganic surfaces from time-dependent density functional theory calculations. Physical Chemistry Chemical Physics, 2011, 13, 15055.	2.8	5
169	Representability problem of density functional theory for superconductors. Physical Review B, 2019, 99, .	3.2	5
170	Halogen molecular modifications at high pressure: the case of iodine. Physical Chemistry Chemical Physics, 2021, 23, 3321-3326.	2.8	5
171	Defect levels from SCAN and MBJ meta-GGA exchange-correlation potentials. Physical Review B, 2021, 104, .	3.2	5
172	Photoabsorption spectra of small cationic xenon clusters from time-dependent density functional theory. Journal of Chemical Physics, 2009, 131, 214302.	3.0	4
173	Comment on â€œTopological Insulators in Ternary Compounds with a Honeycomb Latticeâ€• Physical Review Letters, 2013, 110, 129701.	7.8	4
174	Meta-Local Density Functionals: A New Rung on Jacobâ€™s Ladder. Journal of Chemical Theory and Computation, 2021, 17, 943-948.	5.3	4
175	A Global-Optimization Study of the Phase Diagram of Free-Standing Hydrogenated Two-Dimensional Silicon. Journal of Physical Chemistry C, 2021, 125, 6298-6305.	3.1	4
176	Point defects in hexagonal silicon. Physical Review Materials, 2021, 5, .	2.4	4
177	Size-dependent optical absorption of Cu2ZnSn(Se,S)4 quantum dot sensitizers from ab initio many-body methods. European Physical Journal B, 2018, 91, 1.	1.5	3
178	Authorship and citation cultural nature in Density Functional Theory from solid state computational packages. Scientometrics, 2021, 126, 6681-6695.	3.0	3
179	Two-dimensional binary metal-oxide quasicrystal approximants. 2D Materials, 2021, 8, 045002.	4.4	3
180	Structure, Magnetism, and Thermal Stability of La₂NiO_{2.5}F₃: A Ruddlesdenâ€“Popper Oxyfluoride Crystallizing in Space Group P4₂/nnm. Inorganic Chemistry, 2021, 60, 13646-13657.	4.0	3

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