Miguel A L Marques

List of Publications by Year in Descending Order

181 papers	10,765 citations	49 h-index	100 g-index
199 ext. papers	12,582 ext. citations	5 avg, IF	6.65 L-index

#	Paper	IF	Citations
181	A dataset of 175k stable and metastable materials calculated with the PBEsol and SCAN functionals.. *Scientific Data*, **2022**, 9, 64	8.2	1
180	Crystal graph attention networks for the prediction of stable materials. *Science Advances*, **2021**, 7, eabi7948	14.3	5
179	A Global-Optimization Study of the Phase Diagram of Free-Standing Hydrogenated Two-Dimensional Silicon. *Journal of Physical Chemistry C*, **2021**, 125, 6298-6305	3.8	4
178	Atomically Thin Pythagorean Tilings in Two Dimensions. *Journal of Physical Chemistry Letters*, **2021**, 12, 4972-4979	6.4	2
177	Authorship and citation cultural nature in Density Functional Theory from solid state computational packages. *Scientometrics*, **2021**, 126, 6681-6695	3	0
176	Two-dimensional binary metal-oxide quasicrystal approximants. *2D Materials*, **2021**, 8, 045002	5.9	1
175	Electronic Structure of Molecules, Surfaces, and Molecules on Surfaces with the Local Modified Becke-Johnson Exchange-Correlation Potential. *Journal of Chemical Theory and Computation*, **2021**, 17, 4746-4755	6.4	3
174	Bishop'S hat silicene: a planar square silicon bilayer decorated with adatoms. *Physical Chemistry Chemical Physics*, **2021**, 23, 16942-16947	3.6	
173	A high-throughput study of oxynitride, oxyfluoride and nitrofluoride perovskites. *Journal of Materials Chemistry A*, **2021**, 9, 8501-8513	13	7
172	Predicting stable crystalline compounds using chemical similarity. *Npj Computational Materials*, **2021**, 7,	10.9	8
171	Halogen molecular modifications at high pressure: the case of iodine. *Physical Chemistry Chemical Physics*, **2021**, 23, 3321-3326	3.6	2
170	Meta-Local Density Functionals: A New Rung on Jacob'S Ladder. *Journal of Chemical Theory and Computation*, **2021**, 17, 943-948	6.4	0
169	Direct insight into the structure-property relation of interfaces from constrained crystal structure prediction. *Nature Communications*, **2021**, 12, 811	17.4	1
168	First-Principles Identification of Single Photon Emitters Based on Carbon Clusters in Hexagonal Boron Nitride. *Journal of Physical Chemistry A*, **2021**, 125, 1325-1335	2.8	14
167	Structure, Magnetism, and Thermal Stability of LaNiOF: A Ruddlesden-Popper Oxyfluoride Crystallizing in Space Group 4/. *Inorganic Chemistry*, **2021**, 60, 13646-13657	5.1	1
166	Bandgap of two-dimensional materials: Thorough assessment of modern exchange-correlation functionals. *Journal of Chemical Physics*, **2021**, 155, 104103	3.9	4
165	Superior carbon nanotube stability by molecular filling:a single-chirality study at extreme pressures. *Carbon*, **2021**, 183, 884-892	10.4	2

164	Reduced Density Matrix Functional Theory for Bosons. *Physical Review Letters*, **2020**, 124, 180603	7.4	9
163	Validation of Pseudopotential Calculations for the Electronic Band Gap of Solids. *Journal of Chemical Theory and Computation*, **2020**, 16, 3620-3627	6.4	9
162	Octopus, a computational framework for exploring light-driven phenomena and quantum dynamics in extended and finite systems. *Journal of Chemical Physics*, **2020**, 152, 124119	3.9	86
161	Accurate electronic band gaps of two-dimensional materials from the local modified Becke-Johnson potential. *Physical Review B*, **2020**, 101,	3.3	8
160	Local Modified Becke-Johnson Exchange-Correlation Potential for Interfaces, Surfaces, and Two-Dimensional Materials. *Journal of Chemical Theory and Computation*, **2020**, 16, 2654-2660	6.4	15
159	Advanced Raman spectroscopy of Cs2AgBiBr6 double perovskites and identification of Cs3Bi2Br9 secondary phases. *Scripta Materialia*, **2020**, 184, 24-29	5.6	17
158	Novel two-dimensional silicon-carbon binaries by crystal structure prediction. *Physical Chemistry Chemical Physics*, **2020**, 22, 8442-8449	3.6	5
157	Tight-Binding Parameterizations of Ti and Ba Oxides and Their Application for the Prediction of 2D Phases. *Physica Status Solidi (B): Basic Research*, **2020**, 257, 1900634	1.3	2
156	The Abinitproject: Impact, environment and recent developments. *Computer Physics Communications*, **2020**, 248, 107042	4.2	143
155	The CECAM electronic structure library and the modular software development paradigm. *Journal of Chemical Physics*, **2020**, 153, 024117	3.9	5
154	Exchange-correlation functionals for band gaps of solids: benchmark, reparametrization and machine learning. *Npj Computational Materials*, **2020**, 6,	10.9	63
153	Stable Ordered Phases of Cuprous Iodide with Complexes of Copper Vacancies. *Chemistry of Materials*, **2019**, 31, 7877-7882	9.6	10
152	Semilocal exchange-correlation potentials for solid-state calculations: Current status and future directions. *Journal of Applied Physics*, **2019**, 126, 110902	2.5	21
151	Double perovskites as p-type conducting transparent semiconductors: a high-throughput search. *Journal of Materials Chemistry A*, **2019**, 7, 14705-14711	13	15
150	Structural prediction of stabilized atomically thin tin layers. *Npj 2D Materials and Applications*, **2019**, 3,	8.8	11
149	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	3.6	16
148	Rare-earth magnetic nitride perovskites. *JPhys Materials*, **2019**, 2, 025003	4.2	14
147	Recent advances and applications of machine learning in solid-state materials science. *Npj Computational Materials*, **2019**, 5,	10.9	631

146	On the time evolution of fermionic occupation numbers. *Journal of Chemical Physics*, **2019**, 151, 044112	3.9	8
145	Large-Scale Benchmark of Exchange-Correlation Functionals for the Determination of Electronic Band Gaps of Solids. *Journal of Chemical Theory and Computation*, **2019**, 15, 5069-5079	6.4	92
144	Computational acceleration of prospective dopant discovery in cuprous iodide. *Physical Chemistry Chemical Physics*, **2019**, 21, 18839-18849	3.6	21
143	Mechanism of surface passivation of methylammonium lead tribromide single crystals by benzylamine. *Applied Physics Reviews*, **2019**, 6, 031401	17.3	28
142	Reduced density matrix functional theory for superconductors. *Physical Review B*, **2019**, 99,	3.3	9
141	Machine Learning the Physical Nonlocal Exchange-Correlation Functional of Density-Functional Theory. *Journal of Physical Chemistry Letters*, **2019**, 10, 6425-6431	6.4	34
140	On the calculation of the bandgap of periodic solids with MGGA functionals using the total energy. *Journal of Chemical Physics*, **2019**, 151, 161102	3.9	5
139	Representability problem of density functional theory for superconductors. *Physical Review B*, **2019**, 99,	3.3	5
138	Stable hybrid organic□inorganic halide perovskites for photovoltaics from ab initio high-throughput calculations. *Journal of Materials Chemistry A*, **2018**, 6, 6463-6475	13	33
137	Propagators for the Time-Dependent Kohn-Sham Equations: Multistep, Runge-Kutta, Exponential Runge-Kutta, and Commutator Free Magnus Methods. *Journal of Chemical Theory and Computation*, **2018**, 14, 3040-3052	6.4	44
136	High-pressure phases of VO2 from the combination of Raman scattering and ab initio structural search. *Physical Review B*, **2018**, 97,	3.3	7
135	Local Hybrid Density Functional for Interfaces. *Journal of Chemical Theory and Computation*, **2018**, 14, 939-947	6.4	16
134	The ground state of two-dimensional silicon. *2D Materials*, **2018**, 5, 035010	5.9	21
133	Efficient Automatized Density-Functional Tight-Binding Parametrizations: Application to Group IV Elements. *Journal of Chemical Theory and Computation*, **2018**, 14, 2947-2954	6.4	13
132	Nitrogen-hydrogen-oxygen ternary phase diagram: New phases at high pressure from structural prediction. *Physical Review Materials*, **2018**, 2,	3.2	12
131	Recent developments in libxc □A comprehensive library of functionals for density functional theory. *SoftwareX*, **2018**, 7, 1-5	2.7	180
130	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	1.2	2
129	Predicting the stability of ternary intermetallics with density functional theory and machine learning. *Journal of Chemical Physics*, **2018**, 148, 241728	3.9	18

128	Static correlated functionals for reduced density matrix functional theory. *European Physical Journal B*, **2018**, 91, 1	1.2	9
127	Predicting the Thermodynamic Stability of Solids Combining Density Functional Theory and Machine Learning. *Chemistry of Materials*, **2017**, 29, 5090-5103	9.6	144
126	Towards a formal definition of static and dynamic electronic correlations. *Physical Chemistry Chemical Physics*, **2017**, 19, 12655-12664	3.6	28
125	High-throughput search of ternary chalcogenides for p-type transparent electrodes. *Scientific Reports*, **2017**, 7, 43179	4.9	36
124	Pressure-induced radial collapse in few-wall carbon nanotubes: A combined theoretical and experimental study. *Carbon*, **2017**, 125, 429-436	10.4	23
123	From mesoscale to nanoscale mechanics in single-wall carbon nanotubes. *Carbon*, **2017**, 123, 145-150	10.4	30
122	Emergence of superconductivity in doped HO ice at high pressure. *Scientific Reports*, **2017**, 7, 6825	4.9	19
121	Structural prediction of two-dimensional materials under strain. *2D Materials*, **2017**, 4, 045009	5.9	17
120	Relating correlation measures: The importance of the energy gap. *Physical Review A*, **2017**, 95,	2.6	13
119	Optimization of the ionization time of an atom with tailored laser pulses: a theoretical study. *European Physical Journal B*, **2017**, 90, 1	1.2	1
118	Novel crystal structures for lithium–silicon alloy predicted by minima hopping method. *Journal of Alloys and Compounds*, **2016**, 655, 147-154	5.7	17
117	Topological Crystalline Insulator in a New Bi Semiconducting Phase. *Scientific Reports*, **2016**, 6, 21790	4.9	9
116	The optimal one dimensional periodic table: a modified Pettifor chemical scale from data mining. *New Journal of Physics*, **2016**, 18, 093011	2.9	30
115	Investigation of new phases in the Ba-Si phase diagram under high pressure using ab initio structural search. *Physical Chemistry Chemical Physics*, **2016**, 18, 8108-14	3.6	10
114	Stability and electronic properties of new inorganic perovskites from high-throughput ab initio calculations. *Journal of Materials Chemistry C*, **2016**, 4, 3157-3167	7.1	156
113	Nanostructured water and carbon dioxide inside collapsing carbon nanotubes at high pressure. *Physical Chemistry Chemical Physics*, **2016**, 18, 19926-32	3.6	15
112	Research Update: Stable single-phase Zn-rich Cu2ZnSnSe4 through In doping. *APL Materials*, **2016**, 4, 070701	5.7	9
111	Prediction and Synthesis of a Non-Zintl Silicon Clathrate. *Chemistry of Materials*, **2016**, 28, 3711-3717	9.6	8

110	Radial collapse of carbon nanotubes for conductivity optimized polymer composites. *Carbon*, **2016**, 106, 64-73	10.4	23
109	Optical properties of Cu-chalcogenide photovoltaic absorbers from self-consistent GW and the Bethe-Salpeter equation. *Physical Review B*, **2015**, 91,	3.3	16
108	Identification of Novel Cu, Ag, and Au Ternary Oxides from Global Structural Prediction. *Chemistry of Materials*, **2015**, 27, 4562-4573	9.6	47
107	Superconductivity in an expanded phase of ZnO: anab initiostudy. *New Journal of Physics*, **2015**, 17, 043024	2.9	9
106	Optimized Exchange and Correlation Semilocal Functional for the Calculation of Energies of Formation. *Journal of Chemical Theory and Computation*, **2015**, 11, 3844-50	6.4	18
105	Insights into colour-tuning of chlorophyll optical response in green plants. *Physical Chemistry Chemical Physics*, **2015**, 17, 26599-606	3.6	37
104	Materials Design On-the-Fly. *Journal of Chemical Theory and Computation*, **2015**, 11, 3955-60	6.4	24
103	Novel phases of lithium-aluminum binaries from first-principles structural search. *Journal of Chemical Physics*, **2015**, 142, 024710	3.9	12
102	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, 31371-96	3.6	276
101	Generalized Pauli constraints in reduced density matrix functional theory. *Journal of Chemical Physics*, **2015**, 142, 154108	3.9	35
100	Prediction of Stable Nitride Perovskites. *Chemistry of Materials*, **2015**, 27, 5957-5963	9.6	75
99	Low-density silicon allotropes for photovoltaic applications. *Physical Review B*, **2015**, 92,	3.3	58
98	Detection of Cu2Zn5SnSe8 and Cu2Zn6SnSe9 phases in co-evaporated Cu2ZnSnSe4 thin-films. *Applied Physics Letters*, **2015**, 107, 172102	3.4	5
97	Accuracy of generalized gradient approximation functionals for density-functional perturbation theory calculations. *Physical Review B*, **2014**, 89,	3.3	119
96	Ab initio calculations of the ground and excited states of the YN molecule including spin□orbit effects. *Chemical Physics*, **2014**, 429, 33-43	2.3	7
95	Benchmark Many-Body GW and Bethe-Salpeter Calculations for Small Transition Metal Molecules. *Journal of Chemical Theory and Computation*, **2014**, 10, 3934-43	6.4	87
94	Construction of the B88 Exchange-Energy Functional in Two Dimensions. *Journal of Chemical Theory and Computation*, **2014**, 10, 1837-42	6.4	14
93	Density-functional tight-binding study of the collapse of carbon nanotubes under hydrostatic pressure. *Carbon*, **2014**, 69, 355-360	10.4	36

92	Comment on "Towards direct-gap silicon phases by the inverse band structure design approach". *Physical Review Letters*, **2014**, 112, 199801	7.4	2
91	First-principles predicted low-energy structures of NaSc(BH4)4. *Journal of Chemical Physics*, **2014**, 140, 124708	3.9	17
90	Benchmarking the AK13 Exchange Functional: Ionization Potentials and Electron Affinities. *Journal of Chemical Theory and Computation*, **2014**, 10, 5625-9	6.4	15
89	Probing time-dependent molecular dipoles on the attosecond time scale. *Physical Review Letters*, **2013**, 111, 033001	7.4	89
88	Carbon structures and defect planes in diamond at high pressure. *Physical Review B*, **2013**, 88,	3.3	30
87	Full color modulation of firefly luciferase through engineering with unified Stark effect. *Journal of Physical Chemistry B*, **2013**, 117, 13725-30	3.4	18
86	Prediction of a novel monoclinic carbon allotrope. *European Physical Journal B*, **2013**, 86, 1	1.2	13
85	Benchmarking the Starting Points of the GW Approximation for Molecules. *Journal of Chemical Theory and Computation*, **2013**, 9, 324-9	6.4	182
84	Conducting boron sheets formed by the reconstruction of the □boron (111) surface. *Physical Review Letters*, **2013**, 111, 136101	7.4	39
83	Comment on "Topological insulators in ternary compounds with a honeycomb lattice". *Physical Review Letters*, **2013**, 110, 129701	7.4	4
82	Ab Initio Electronic Gaps of Ge Nanodots: The Role of Self-Energy Effects. *Journal of Physical Chemistry C*, **2013**, 117, 14229-14234	3.8	10
81	Atomic and electronic properties of quasi-one-dimensional MOS nanowires. *Journal of Materials Research*, **2013**, 28, 240-249	2.5	16
80	Sodium□old binaries: novel structures for ionic compounds from anab initiostructural search. *New Journal of Physics*, **2013**, 15, 115007	2.9	36
79	Strong renormalization of the electronic band gap due to lattice polarization in the GW formalism. *Physical Review Letters*, **2013**, 110, 226404	7.4	51
78	Low-energy polymeric phases of alanates. *Physical Review Letters*, **2013**, 110, 135502	7.4	33
77	The crystal structure of p-type transparent conductive oxide CuBO2. *MRS Communications*, **2013**, 3, 157-160	1.7	10
76	Response Functions in TDDFT: Concepts and Implementation. *Lecture Notes in Physics*, **2012**, 139-166	0.8	11
75	Violation of a local form of the Lieb-Oxford bound. *Physical Review A*, **2012**, 85,	2.6	10

74	Ab initio angle- and energy-resolved photoelectron spectroscopy with time-dependent density-functional theory. *Physical Review A*, **2012**, 85,	2.6	74
73	Libxc: A library of exchange and correlation functionals for density functional theory. *Computer Physics Communications*, **2012**, 183, 2272-2281	4.2	323
72	Low-energy silicon allotropes with strong absorption in the visible for photovoltaic applications. *Physical Review B*, **2012**, 86,	3.3	116
71	p doping in expanded phases of ZnO: an ab initio study. *Physical Review Letters*, **2012**, 108, 115903	7.4	18
70	Speeding up the solution of the Bethe-Salpeter equation by a double-grid method and Wannier interpolation. *Physical Review B*, **2012**, 86,	3.3	34
69	High-pressure structures of disilane and their superconducting properties. *Physical Review Letters*, **2012**, 108, 117004	7.4	80
68	Raman activity of sp3 carbon allotropes under pressure: A density functional theory study. *Physical Review B*, **2012**, 85,	3.3	25
67	Time-dependent density-functional theory in massively parallel computer architectures: the OCTOPUS project. *Journal of Physics Condensed Matter*, **2012**, 24, 233202	1.8	135
66	Novel structural motifs in low energy phases of LiAlH4. *Physical Review Letters*, **2012**, 108, 205505	7.4	42
65	Crystal structure of cold compressed graphite. *Physical Review Letters*, **2012**, 108, 065501	7.4	265
64	Kirzhnits gradient expansion in two dimensions. *Physical Review B*, **2012**, 85,	3.3	19
63	Band structures of Cu2ZnSnS4 and Cu2ZnSnSe4 from many-body methods. *Applied Physics Letters*, **2011**, 98, 241915	3.4	103
62	Density functional theory beyond the linear regime: Validating an adiabatic local density approximation. *Physical Review A*, **2011**, 83,	2.6	54
61	Density-based mixing parameter for hybrid functionals. *Physical Review B*, **2011**, 83,	3.3	290
60	Modeling van der Waals interactions between proteins and inorganic surfaces from time-dependent density functional theory calculations. *Physical Chemistry Chemical Physics*, **2011**, 13, 15055-61	3.6	5
59	Simple preconditioning for time-dependent density functional perturbation theory. *Journal of Chemical Physics*, **2011**, 135, 014103	3.9	6
58	Accurate color tuning of firefly chromophore by modulation of local polarization electrostatic fields. *Journal of Physical Chemistry B*, **2011**, 115, 329-32	3.4	35
57	Optimal control of the electronic current density: Application to one- and two-dimensional one-electron systems. *Physical Review A*, **2011**, 83,	2.6	6

56	Enhancing the superconducting transition temperature of BaSi2 by structural tuning. *Physical Review Letters*, **2011**, 106, 087002	7.4	17
55	Superconductivity in layered binary silicides: A density functional theory study. *Physical Review B*, **2011**, 84,	3.3	18
54	Band structures of delafossite transparent conductive oxides from a self-consistent GW approach. *Physical Review B*, **2010**, 82,	3.3	57
53	Effects of electronic and lattice polarization on the band structure of delafossite transparent conductive oxides. *Physical Review Letters*, **2010**, 104, 136401	7.4	83
52	Excitonic effects in the optical properties of CdSe nanowires. *Applied Physics Letters*, **2010**, 96, 123106	3.4	23
51	Toward an All-Around Semilocal Potential for Electronic Exchange. *Journal of Chemical Theory and Computation*, **2010**, 6, 3664-3670	6.4	17
50	Fragment molecular orbital investigation of the role of AMP protonation in firefly luciferase pH-sensitivity. *Physical Chemistry Chemical Physics*, **2010**, 12, 14285-93	3.6	46
49	Bioheterojunction Effect on Fluorescence Origin and Efficiency Improvement of Firefly Chromophores. *Journal of Physical Chemistry Letters*, **2010**, 1, 2781-2787	6.4	29
48	Alloying effects on the optical properties of Ge1−xSix nanocrystals from time-dependent density functional theory and comparison with effective-medium theory. *Physical Review B*, **2009**, 79,	3.3	5
47	Photoabsorption spectra of small cationic xenon clusters from time-dependent density functional theory. *Journal of Chemical Physics*, **2009**, 131, 214302	3.9	4
46	Density gradients for the exchange energy of electrons in two dimensions. *Physical Review A*, **2009**, 79,	2.6	28
45	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	1.4	19
44	Towards a gauge invariant method for molecular chiroptical properties in TDDFT. *Physical Chemistry Chemical Physics*, **2009**, 11, 4481-9	3.6	38
43	Optical and magnetic properties of boron fullerenes. *Physical Chemistry Chemical Physics*, **2009**, 11, 4523-36	3.6	43
42	Density-matrix-power functional: Performance for finite systems and the homogeneous electron gas. *Physical Review A*, **2009**, 79,	2.6	80
41	Local correlation functional for electrons in two dimensions. *Physical Review B*, **2008**, 78,	3.3	24
40	Specification of an extensible and portable file format for electronic structure and crystallographic data. *Computational Materials Science*, **2008**, 43, 1056-1065	3.2	5
39	Benchmark calculations for reduced density-matrix functional theory. *Journal of Chemical Physics*, **2008**, 128, 184103	3.9	65

38	The role of dimensionality on the quenching of spin-orbit effects in the optics of gold nanostructures. *Journal of Chemical Physics*, **2008**, 129, 144110	3.9	33
37	Empirical functionals for reduced-density-matrix-functional theory. *Physical Review A*, **2008**, 77,	2.6	71
36	Cluster-surface and cluster-cluster interactions: Ab initio calculations and modeling of asymptotic van der Waals forces. *Physical Review B*, **2008**, 78,	3.3	23
35	On the use of Neumann's principle for the calculation of the polarizability tensor of nanostructures. *Journal of Nanoscience and Nanotechnology*, **2008**, 8, 3392-8	1.3	14
34	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	3.9	28
33	Superconducting properties of MgB2 from first principles. *Physica C: Superconductivity and Its Applications*, **2007**, 456, 45-53	1.3	37
32	Identification of fullerene-like CdSe nanoparticles from optical spectroscopy calculations. *Physical Review B*, **2007**, 75,	3.3	45
31	Time-dependent density functional theory scheme for efficient calculations of dynamic (hyper)polarizabilities. *Journal of Chemical Physics*, **2007**, 126, 184106	3.9	94
30	Molecules and clusters in strong laser fields **2007**, 485-617		2
29	Superconductivity in lithium, potassium, and aluminum under extreme pressure: a first-principles study. *Physical Review Letters*, **2006**, 96, 047003	7.4	138
28	A TDDFT study of the excited states of DNA bases and their assemblies. *Journal of Physical Chemistry B*, **2006**, 110, 7129-38	3.4	104
27	Magnetic response and NMR spectra of carbon nanotubes from ab initio calculations. *Physical Review B*, **2006**, 73,	3.3	66
26	Ab initio prediction of pressure-induced superconductivity in potassium. *Physical Review B*, **2006**, 73,	3.3	37
25	octopus: a tool for the application of time-dependent density functional theory. *Physica Status Solidi (B): Basic Research*, **2006**, 243, 2465-2488	1.3	659
24	Optical absorption of the blue fluorescent protein: a first-principles study. *Journal of the American Chemical Society*, **2005**, 127, 12329-37	16.4	66
23	Ab initio theory of superconductivity. II. Application to elemental metals. *Physical Review B*, **2005**, 72,	3.3	199
22	Ab initio theory of superconductivity. I. Density functional formalism and approximate functionals. *Physical Review B*, **2005**, 72,	3.3	237
21	A viable way to tailor carbon nanomaterials by irradiation-induced transformations. *Radiation Physics and Chemistry*, **2005**, 73, 334-339	2.5	13

20	Ab-initio Computation of Superconducting Properties of Elemental Superconductors and MgB2. *Journal of Superconductivity and Novel Magnetism*, **2005**, 18, 649-652		1
19	Time-dependent electron localization function. *Physical Review A*, **2005**, 71,	2.6	101
18	Superconducting properties of MgB2 from first principles. *Physical Review Letters*, **2005**, 94, 037004	7.4	122
17	The planar-to-tubular structural transition in boron clusters from optical absorption. *Journal of Chemical Physics*, **2005**, 123, 014310	3.9	45
16	Excited states dynamics in time-dependent density functional theory. *European Physical Journal D*, **2004**, 28, 211-218	1.3	114
15	Time-dependent density functional theory. *Annual Review of Physical Chemistry*, **2004**, 55, 427-55	15.7	932
14	Density functional theory for superconductors. *International Journal of Quantum Chemistry*, **2004**, 99, 790-797	2.1	14
13	On the Breaking of Carbon Nanotubes under Tension. *Nano Letters*, **2004**, 4, 811-815	11.5	87
12	Propagators for the time-dependent Kohn-Sham equations. *Journal of Chemical Physics*, **2004**, 121, 3425-33	3.9	403
11	Time and energy-resolved two photon photoemission of the Cu(1 0 0) and Cu(1 1 1) metal surfaces. *Computational Materials Science*, **2004**, 30, 110-115	3.2	10
10	An Application of Non-Extensive Statistical Mechanics to Nanosystems. *Journal of Computational and Theoretical Nanoscience*, **2004**, 1, 227-229	0.3	40
9	Optical Properties of Nanostructures from Time-Dependent Density Functional Theory. *Journal of Computational and Theoretical Nanoscience*, **2004**, 1, 231-255	0.3	17
8	octopus: a first-principles tool for excited electron–ion dynamics. *Computer Physics Communications* , **2003**, 151, 60-78	4.2	569
7	Direct Observation of the Mechanical Properties of Single-Walled Carbon Nanotubes and Their Junctions at the Atomic Level. *Nano Letters*, **2003**, 3, 751-755	11.5	135
6	A Tutorial on Density Functional Theory. *Lecture Notes in Physics*, **2003**, 218-256	0.8	23
5	Time-dependent density-functional approach for biological chromophores: the case of the green fluorescent protein. *Physical Review Letters*, **2003**, 90, 258101	7.4	166
4	Time-Dependent Density Functional Theory. *Lecture Notes in Physics*, **2003**, 144-184	0.8	50
3	Can optical spectroscopy directly elucidate the ground state of C20?. *Journal of Chemical Physics*, **2002**, 116, 1930-1933	3.9	51

2	Roadmap on Machine Learning in Electronic Structure. *Electronic Structure*,	2.6	7
1	Machine-learning correction to density-functional crystal structure optimization. *MRS Bulletin*,1	3.2	1