Micael J T Oliveira

List of Publications by Year
in descending order

31 papers	6,426 citations	361413 20 h-index	454955 30 g-index
31 all docs	31 docs citations	31 times ranked	6704 citing authors

#	Article	IF	Citations
1	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	7.5	2,297
2	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
3	Recent developments in the ABINIT software package. Computer Physics Communications, 2016, 205, 106-131.	7.5	662
4	Libxc: A library of exchange and correlation functionals for density functional theory. Computer Physics Communications, 2012, 183, 2272-2281.	7.5	419
5	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
6	Recent developments in libxc â€" A comprehensive library of functionals for density functional theory. SoftwareX, 2018, 7, 1-5.	2.6	367
7	Density-based mixing parameter for hybrid functionals. Physical Review B, 2011, 83, .	3.2	338
8	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
9	Time-dependent density-functional theory in massively parallel computer architectures: the octopus project. Journal of Physics Condensed Matter, 2012, 24, 233202.	1.8	181
10	Accuracy of generalized gradient approximation functionals for density-functional perturbation theory calculations. Physical Review B, 2014, 89, .	3.2	138
11	Generating relativistic pseudo-potentials with explicit incorporation of semi-core states using APE, the Atomic Pseudo-potentials Engine. Computer Physics Communications, 2008, 178, 524-534.	7.5	125
12	Band widths and gaps from the Tran-Blaha functional: Comparison with many-body perturbation theory. Physical Review B, 2013, 87, .	3.2	125
13	Towards efficient data exchange and sharing for big-data driven materials science: metadata and data formats. Npj Computational Materials, 2017, 3, .	8.7	79
14	Light-matter interactions within the Ehrenfestâ€"Maxwellâ€"Pauliâ€"Kohnâ€"Sham framework: fundamentals, implementation, and nano-optical applications. Advances in Physics, 2019, 68, 225-333.	14.4	54
15	Insights into colour-tuning of chlorophyll optical response in green plants. Physical Chemistry Chemical Physics, 2015, 17, 26599-26606.	2.8	46
16	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
17	Self-consistent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:math> method for real-space time-dependent density functional theory calculations. Physical Review B, 2017, 96, .	3.2	35
18	Time-dependent density-functional theory of strong-field ionization of atoms by soft x rays. Physical Review A, 2014, 90, .	2.5	29

#	Article	IF	Citations
19	Optical and Magnetic Excitations of Metal-Encapsulating Si Cages: A Systematic Study by Time-Dependent Density Functional Theory. Journal of Physical Chemistry C, 2014, 118, 11377-11384.	3.1	25
20	A survey of the parallel performance and accuracy of Poisson solvers for electronic structure calculations. Journal of Computational Chemistry, 2014, 35, 427-444.	3.3	23
21	Toward an All-Around Semilocal Potential for Electronic Exchange. Journal of Chemical Theory and Computation, 2010, 6, 3664-3670.	5.3	19
22	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
23	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
24	Benchmarking the AK13 Exchange Functional: Ionization Potentials and Electron Affinities. Journal of Chemical Theory and Computation, 2014, 10, 5625-5629.	5.3	15
25	Computational Benchmarking for Ultrafast Electron Dynamics: Wave Function Methods vs Density Functional Theory. Journal of Chemical Theory and Computation, 2015, 11, 2221-2233.	5.3	11
26	Finite-Size Effects in the Absorption Spectra of a Single-Wall Carbon Nanotube. Journal of Physical Chemistry C, 2016, 120, 18268-18274.	3.1	9
27	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
28	Photoabsorption spectra of small cationic xenon clusters from time-dependent density functional theory. Journal of Chemical Physics, 2009, 131, 214302.	3.0	4
29	Spinâ€“orbit effects in the bismuth atom and dimer: tight-binding and density functional theory comparison. Journal of Physics B: Atomic, Molecular and Optical Physics, 2013, 46, 095101.	1.5	4
30	Recent Memory and Performance Improvements in Octopus Code. Lecture Notes in Computer Science, 2014, , 607-622.	1.3	3
31	First-principles characterisation of spectroscopic and bonding properties of cationic bismuth carbide clusters. Computational and Theoretical Chemistry, 2021, 1204, 113372.	2.5	0