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	First-principles characterisation of spectroscopic and bonding properties of cationic bismuth carbide clusters. Computational and Theoretical Chemistry, 2021, 1204, 113372.	2.5	0
2	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
3	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
4	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
5	Recent developments in libxc â€” A comprehensive library of functionals for density functional theory. SoftwareX, 2018, 7, 1-5.	2.6	367
6	Towards efficient data exchange and sharing for big-data driven materials science: metadata and data formats. Npj Computational Materials, 2017, 3, .	8.7	79
7	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
8	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
9	Recent developments in the ABINIT software package. Computer Physics Communications, 2016, 205, 106-131.	7.5	662
10	Insights into colour-tuning of chlorophyll optical response in green plants. Physical Chemistry Chemical Physics, 2015, 17, 26599-26606.	2.8	46
11	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
12	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
13	Recent Memory and Performance Improvements in Octopus Code. Lecture Notes in Computer Science, 2014, , 607-622.	1.3	3
14	Benchmarking the AK13 Exchange Functional: Ionization Potentials and Electron Affinities. Journal of Chemical Theory and Computation, 2014, 10, 5625-5629.	5.3	15
15	Accuracy of generalized gradient approximation functionals for density-functional perturbation theory calculations. Physical Review B, 2014, 89, .	3.2	138
16	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
17	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
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	Band widths and gaps from the Tran-Blaha functional: Comparison with many-body perturbation theory. Physical Review B, 2013, 87, .	3.2	125
20	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
21	Libxc: A library of exchange and correlation functionals for density functional theory. Computer Physics Communications, 2012, 183, 2272-2281.	7.5	419
22	Time-dependent density-functional theory in massively parallel computer architectures: the octopus project. Journal of Physics Condensed Matter, 2012, 24, 233202.	1.8	181
23	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
24	Density-based mixing parameter for hybrid functionals. Physical Review B, 2011, 83, .	3.2	338
25	Toward an All-Around Semilocal Potential for Electronic Exchange. Journal of Chemical Theory and Computation, 2010, 6, 3664-3670.	5.3	19
26	Photoabsorption spectra of small cationic xenon clusters from time-dependent density functional theory. Journal of Chemical Physics, 2009, 131, 214302.	3.0	4
27	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	7.5	2,297
28	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
29	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
30	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
31	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