

Xavier Andrade

List of Publications by Year in descending order

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Version: 2024-02-01

30
papers

2,410
citations

394421

19
h-index

477307

29
g-index

32
all docs

32
docs citations

32
times ranked

2309
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	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
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	Time-dependent density-functional theory in massively parallel computer architectures: the octopus project. Journal of Physics Condensed Matter, 2012, 24, 233202.	1.8	181
5	Modified Ehrenfest Formalism for Efficient Large-Scale ab initio Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 728-742.	5.3	124
6	Time-dependent density functional theory scheme for efficient calculations of dynamic (hyper)polarizabilities. Journal of Chemical Physics, 2007, 126, 184106.	3.0	106
7	Real-Space Density Functional Theory on Graphical Processing Units: Computational Approach and Comparison to Gaussian Basis Set Methods. Journal of Chemical Theory and Computation, 2013, 9, 4360-4373.	5.3	53
8	Theoretical investigation of free-standing CoPd nanoclusters as a function of cluster size and stoichiometry in the Pd-rich phase: Geometry, chemical order, magnetism, and metallic behavior. Physical Review B, 2006, 74, .	3.2	52
9	Prediction of the Derivative Discontinuity in Density Functional Theory from an Electrostatic Description of the Exchange and Correlation Potential. Physical Review Letters, 2011, 107, 183002.	7.8	52
10	Optical and magnetic properties of boron fullerenes. Physical Chemistry Chemical Physics, 2009, 11, 4523.	2.8	50
11	Compressed Sensing for Multidimensional Spectroscopy Experiments. Journal of Physical Chemistry Letters, 2012, 3, 2697-2702.	4.6	50
12	Towards a gauge invariant method for molecular chiroptical properties in TDDFT. Physical Chemistry Chemical Physics, 2009, 11, 4481.	2.8	46
13	Basis set effects on the hyperpolarizability of CHCl ₃ : Gaussian-type orbitals, numerical basis sets and real-space grids. Journal of Chemical Physics, 2010, 133, 034111.	3.0	46
14	Insights into colour-tuning of chlorophyll optical response in green plants. Physical Chemistry Chemical Physics, 2015, 17, 26599-26606.	2.8	46
15	Massively parallel first-principles simulation of electron dynamics in materials. Journal of Parallel and Distributed Computing, 2017, 106, 205-214.	4.1	42
16	Application of compressed sensing to the simulation of atomic systems. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 13928-13933.	7.1	40
17	Cluster-surface and cluster-cluster interactions: Ab initio calculations and modeling of asymptotic van der Waals forces. Physical Review B, 2008, 78, .	3.2	26
18	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

#	ARTICLE	IF	CITATIONS
19	Self-interaction effects on charge-transfer collisions. <i>Physical Review A</i> , 2017, 95, .	2.5	20
20	Measurement of the absolute Raman cross section of the optical phonons in type Ia natural diamond. <i>Solid State Communications</i> , 2012, 152, 204-209.	1.9	18
21	Negative differential conductivity in liquid aluminum from real-time quantum simulations. <i>European Physical Journal B</i> , 2018, 91, 1.	1.5	18
22	The structure and properties of small Pd clusters. <i>Nanotechnology</i> , 2008, 19, 205701.	2.6	17
23	Anion Stabilization in Electrostatic Environments. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 682-688.	4.6	14
24	Effect of chemical disorder on the electronic stopping of solid solution alloys. <i>Acta Materialia</i> , 2020, 196, 576-583.	7.9	11
25	Compressed Sensing for the Fast Computation of Matrices: Application to Molecular Vibrations. <i>ACS Central Science</i> , 2015, 1, 24-32.	11.3	8
26	<sc>Inq</sc>, a Modern GPU-Accelerated Computational Framework for (Time-Dependent) Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7447-7467.	5.3	7
27	Harnessing the Power of Graphic Processing Units. <i>Lecture Notes in Physics</i> , 2012, , 401-413.	0.7	6
28	Massively Parallel First-Principles Simulation of Electron Dynamics in Materials. , 2016, , .		5
29	Directional dependency of electronic stopping in nickel, projectileâ€™s excited charge state and momentum transfer. <i>European Physical Journal D</i> , 2021, 75, 1.	1.3	4
30	Accelerating the computation of bath spectral densities with super-resolution. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	2