Xavier Andrade

List of Publications by Year
in descending order

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	Directional dependency of electronic stopping in nickel, projectile's excited charge state and momentum transfer. European Physical Journal D, 2021, 75, 1.	1.3	4
2	<scp>Inq</scp>, a Modern GPU-Accelerated Computational Framework for (Time-Dependent) Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 7447-7467.	5.3	7
3	Effect of chemical disorder on the electronic stopping of solid solution alloys. Acta Materialia, 2020, 196, 576-583.	7.9	11
4	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
5	Negative differential conductivity in liquid aluminum from real-time quantum simulations. European Physical Journal B, 2018, 91, 1.	1.5	18
6	Massively parallel first-principles simulation of electron dynamics in materials. Journal of Parallel and Distributed Computing, 2017, 106, 205-214.	4.1	42
7	Self-interaction effects on charge-transfer collisions. Physical Review A, 2017, 95, .	2.5	20
8	Accelerating the computation of bath spectral densities with super-resolution. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	2
9	Massively Parallel First-Principles Simulation of Electron Dynamics in Materials. , 2016, , .		5
10	Insights into colour-tuning of chlorophyll optical response in green plants. Physical Chemistry Chemical Physics, 2015, 17, 26599-26606.	2.8	46
11	Compressed Sensing for the Fast Computation of Matrices: Application to Molecular Vibrations. ACS Central Science, 2015, 1, 24-32.	11.3	8
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	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
14	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
15	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
16	Compressed Sensing for Multidimensional Spectroscopy Experiments. Journal of Physical Chemistry Letters, 2012, 3, 2697-2702.	4.6	50
17	Time-dependent density-functional theory in massively parallel computer architectures: the octopus project. Journal of Physics Condensed Matter, 2012, 24, 233202.	1.8	181
18	Measurement of the absolute Raman cross section of the optical phonons in type Ia natural diamond. Solid State Communications, 2012, 152, 204-209.	1.9	18

#	Article	IF	Citations
19	Harnessing the Power of Graphic Processing Units. Lecture Notes in Physics, 2012, , 401-413.	0.7	6
20	Anion Stabilization in Electrostatic Environments. Journal of Physical Chemistry Letters, 2011, 2, 682-688.	4.6	14
21	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
22	Basis set effects on the hyperpolarizability of CHCl3: Gaussian-type orbitals, numerical basis sets and real-space grids. Journal of Chemical Physics, 2010, 133, 034111.	3.0	46
23	Modified Ehrenfest Formalism for Efficient Large-Scale ab initio Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 728-742.	5.3	124
24	Towards a gauge invariant method for molecular chiroptical properties in TDDFT. Physical Chemistry Chemical Physics, 2009, 11, 4481.	2.8	46
25	Optical and magnetic properties of boron fullerenes. Physical Chemistry Chemical Physics, 2009, 11, 4523.	2.8	50
26	The structure and properties of small Pd clusters. Nanotechnology, 2008, 19, 205701.	2.6	17
27	Cluster-surface and cluster-cluster interactions:<i>Ab initio</i>calculations and modeling of asymptotic van der Waals forces. Physical Review B, 2008, 78, .	3.2	26
28	Time-dependent density functional theory scheme for efficient calculations of dynamic (hyper)polarizabilities. Journal of Chemical Physics, 2007, 126, 184106.	3.0	106
29	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
30	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