Alberto Castro

List of Publications by Year
in descending order

72 papers	4,760 citations	186265 28 h-index	98798 67 g-index
75 all docs	75 docs citations	75 times ranked	3097 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	octopus: a first-principles tool for excited electronâ€“ion dynamics. Computer Physics Communications, 2003, 151, 60-78.	7.5	671
3	Propagators for the time-dependent Kohnâ€“Sham equations. Journal of Chemical Physics, 2004, 121, 3425-3433.	3.0	477
4	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
5	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
6	Time-Dependent Density-Functional Approach for Biological Chromophores: The Case of the Green Fluorescent Protein. Physical Review Letters, 2003, 90, 258101.	7.8	181
7	Time-dependent density-functional theory in massively parallel computer architectures: the octopus project. Journal of Physics Condensed Matter, 2012, 24, 233202.	1.8	181
8	Assessment of exchange-correlation functionals for the calculation of dynamical properties of small clusters in time-dependent density functional theory. Journal of Chemical Physics, 2001, 115, 3006-3014.	3.0	172
9	Alignment Dependent Ionization of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">N</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>, and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">CO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>	7.8	152
10	Excited states dynamics in time-dependent density functional theory. European Physical Journal D, 2004, 28, 211-218.	1.3	126
11	Modified Ehrenfest Formalism for Efficient Large-Scale ab initio Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 728-742.	5.3	124
12	Optimal Control of Quantum Rings by Terahertz Laser Pulses. Physical Review Letters, 2007, 98, 157404.	7.8	102
13	Single-active-electron approximation for describing molecules in ultrashort laser pulses and its application to molecular hydrogen. Physical Review A, 2008, 77, .	2.5	96
14	Simulating Pumpâ€“Probe Photoelectron and Absorption Spectroscopy on the Attosecond Timescale with Timeâ€Dependent Density Functional Theory. ChemPhysChem, 2013, 14, 1363-1376.	2.1	87
15	Controlling the Dynamics of Many-Electron Systems from First Principles: A Combination of Optimal Control and Time-Dependent Density-Functional Theory. Physical Review Letters, 2012, 109, 153603.	7.8	72
16	Optical Absorption of the Blue Fluorescent Protein: A First-Principles Study. Journal of the American Chemical Society, 2005, 127, 12329-12337.	13.7	69
17	Propagators for the Time-Dependent Kohnâ€“Sham Equations: Multistep, Rungeâ€“Kutta, Exponential Rungeâ€“Kutta, and Commutator Free Magnus Methods. Journal of Chemical Theory and Computation, 2018, 14, 3040-3052.	5.3	69
18	Can optical spectroscopy directly elucidate the ground state of C20?. Journal of Chemical Physics, 2002, 116, 1930-1933.	3.0	55

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19	Optical and magnetic properties of boron fullerenes. Physical Chemistry Chemical Physics, 2009, 11, 4523.	2.8	50
20	A Tutorial on Density Functional Theory. Lecture Notes in Physics, 2003, , 218-256.	0.7	40
21	Scattering of a proton with the Li4 cluster: Non-adiabatic molecular dynamics description based on time-dependent density-functional theory. Chemical Physics, 2012, 399, 130-134.	1.9	40
22	Solution of Poisson's equation for finite systems using plane-wave methods. Canadian Journal of Physics, 2003, 81, 1151-1164.	1.1	39
23	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
24	Water molecules in ultrashort intense laser fields. Chemical Physics, 2013, 414, 45-52.	1.9	36
25	Femtosecond laser pulse shaping for enhanced ionization. Europhysics Letters, 2009, 87, 53001.	2.0	34
26	Enhancing and controlling single-atom high-harmonic generation spectra: a time-dependent density-functional scheme. European Physical Journal B, 2015, 88, 1.	1.5	34
27	Optimal laser control of double quantum dots. Physical Review B, 2008, 77, .	3.2	32
28	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.	3.0	31
29	Optimization schemes for selective molecular cleavage with tailored ultrashort laser pulses. Chemical Physics, 2011, 391, 50-61.	1.9	28
30	Cluster-surface and cluster-cluster interactions:Ab initiocalculations and modeling of asymptotic van der Waals forces. Physical Review B, 2008, 78, .	3.2	26
31	Statistics and NosÃ© formalism for Ehrenfest dynamics. Journal of Physics A: Mathematical and Theoretical, 2011, 44, 395004.	2.1	26
32	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.	0.9	22
33	Optical Properties of Nanostructures from Time-Dependent Density Functional Theory. Journal of Computational and Theoretical Nanoscience, 2004, 1, 231-255.	0.4	21
34	Optimal Control of Molecular Spin Qudits. Physical Review Applied, 2022, 17, .	3.8	21
35	Optimal control of high-harmonic generation by intense few-cycle pulses. Physical Review A, 2014, 90, .	2.5	20
36	Tailored pump-probe transient spectroscopy with time-dependent density-functional theory: controlling absorption spectra. European Physical Journal B, 2016, 89, 1.	1.5	17

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37	Photoabsorption spectra of Ti8C12 metallocarbohedrynes: Theoretical spectroscopy within time-dependent density functional theory. Journal of Chemical Physics, 2006, 125, 074311.	3.0	16
38	Electron localization function for two-dimensional systems. Physical Review B, 2008, 77, .	3.2	16
39	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
40	Exact Coulomb cutoff technique for supercell calculations in two dimensions. Physical Review B, 2009, 80, .	3.2	13
41	Calculation of the optical spectrum of the Ti8C12 and V8C12 Met-Cars. Chemical Physics Letters, 2004, 398, 292-296.	2.6	12
42	Theoretical Shaping of Femtosecond Laser Pulses for Ultrafast Molecular Photoâ€Dissociation with Control Techniques Based on Timeâ€Dependent Density Functional Theory. ChemPhysChem, 2013, 14, 1488-1495.	2.1	12
43	<i>Ab initio</i>molecular dynamics on the electronic Boltzmann equilibrium distribution. New Journal of Physics, 2010, 12, 083064.	2.9	11
44	Optimal control theory for quantum-classical systems: Ehrenfest molecular dynamics based on time-dependent density-functional theory. Journal of Physics A: Mathematical and Theoretical, 2014, 47, 025204.	2.1	11
45	Acceleration of quantum optimal control theory algorithms with mixing strategies. Physical Review E, 2009, 79, 056704.	2.1	10
46	Quantum optimal control theory in the linear response formalism. Physical Review A, 2011, 84, .	2.5	10
47	Ehrenfest Statistical Dynamics in Chemistry: Study of Decoherence Effects. Journal of Chemical Theory and Computation, 2018, 14, 3975-3985.	5.3	8
48	Optical Absorption Spectra of V⁺₄ Isomers: One Example of First-Principles Theoretical Spectroscopy with Time-Dependent Density Functional Theory. Journal of Computational and Theoretical Nanoscience, 2006, 3, 761-766.	0.4	8
49	Single and double charge transfer in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msup><mml:mrow><mml:mi>Ne</mml:mi></mml:mrow><m collision within time-dependent density-functional theory. Physical Review A, 2021, 103, .	2.5	7
50	Coherent quantum switch driven by optimized laser pulses. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 1593-1595.	2.7	6
51	Optimal control of the electronic current density: Application to one- and two-dimensional one-electron systems. Physical Review A, 2011, 83, .	2.5	6
52	Optimal control theory for quantum electrodynamics: an initial state problem. European Physical Journal B, 2019, 92, 1.	1.5	6
53	Non-adiabatic effects within a single thermally averaged potential energy surface: Thermal expansion and reaction rates of small molecules. Journal of Chemical Physics, 2012, 137, 22A533.	3.0	5
54	Shaped electric fields for fast optimal manipulation of electron spin and position in a double quantum dot. Physical Review B, 2016, 93, .	3.2	5

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55	Entropy and canonical ensemble of hybrid quantum classical systems. Physical Review E, 2020, 102, 042118.	2.1	4
56	Theoretical Shaping of Femtosecond Laser Pulses for Molecular Photodissociation with Control Techniques Based on Ehrenfestâ€²s Dynamics and Timeâ€Dependent Density Functional Theory. ChemPhysChem, 2016, 17, 1601-1607.	2.1	3
57	Propagators for Quantum-Classical Models: Commutator-Free Magnus Methods. Journal of Chemical Theory and Computation, 2020, 16, 1420-1430.	5.3	3
58	About the computation of finite temperature ensemble averages of hybrid quantum-classical systems with molecular dynamics. New Journal of Physics, 2021, 23, 063011.	2.9	3
59	Molecules and clusters in strong laser fields. , 2007, , 485-617.		3
60	On the Combination of TDDFT with Molecular Dynamics: New Developments. Lecture Notes in Physics, 2012, , 301-315.	0.7	3
61	CHAPTER 12. Real-time and Real-space Time-dependent Density-functional Theory Approach to Attosecond Dynamics. RSC Theoretical and Computational Chemistry Series, 0, , 424-461.	0.7	3
62	Single-active-electron approximation for molecules in strong laser fields : Test application to H₂. Journal of Physics: Conference Series, 2009, 194, 022064.	0.4	2
63	Ultrafast single electron spin manipulation in 2D semiconductor quantum dots with optimally controlled time-dependent electric fields through spin-orbit coupling. European Physical Journal B, 2015, 88, 1.	1.5	2
64	Nonextensive thermodynamic functions in the SchrÃ¶dinger-Gibbs ensemble. Physical Review E, 2015, 91, 022137.	2.1	2
65	Optimal control with nonadiabatic molecular dynamics: Application to the Coulomb explosion of sodium clusters. Physical Review A, 2016, 94, .	2.5	2
66	About the relation of electronâ€“electron interaction potentials with exchange and correlation functionals. European Physical Journal B, 2018, 91, 1.	1.5	2
67	Quantum Optimal Control. Lecture Notes in Physics, 2012, , 265-276.	0.7	2
68	Optimization of the ionization time of an atom with tailored laser pulses: a theoretical study. European Physical Journal B, 2017, 90, 1.	1.5	1
69	Optimal Control Theory for Electronic Structure Methods. , 2018, , 1-21.		1
70	Density functional study of the structural and electronic properties of aluminium-lithium clusters. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 355-372.	0.2	0
71	Performance of fourth and sixthâ€order commutatorâ€free Magnus expansion integrators for Ehrenfest dynamics. Computational and Mathematical Methods, 2021, 3, e1100.	0.8	0
72	Optimal Control Theory for Electronic Structure Methods. , 2020, , 469-489.		0