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	Optimal Control of Molecular Spin Qudits. Physical Review Applied, 2022, 17, .	3.8	21
2	Performance of fourth and sixthâ€order commutatorâ€free Magnus expansion integrators for Ehrenfest dynamics. Computational and Mathematical Methods, 2021, 3, e1100.	0.8	0
3	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> collision within time-dependent density-functional theory. Physical Review A, 2021, 103, .	2.9	7
4	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
5	Entropy and canonical ensemble of hybrid quantum classical systems. Physical Review E, 2020, 102, 042118.	2.1	4
6	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
7	Propagators for Quantum-Classical Models: Commutator-Free Magnus Methods. Journal of Chemical Theory and Computation, 2020, 16, 1420-1430.	5.3	3
8	Optimal Control Theory for Electronic Structure Methods. , 2020, , 469-489.		0
9	Optimal control theory for quantum electrodynamics: an initial state problem. European Physical Journal B, 2019, 92, 1.	1.5	6
10	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
11	Optimal Control Theory for Electronic Structure Methods. , 2018, , 1-21.		1
12	Ehrenfest Statistical Dynamics in Chemistry: Study of Decoherence Effects. Journal of Chemical Theory and Computation, 2018, 14, 3975-3985.	5.3	8
13	About the relation of electronâ€“electron interaction potentials with exchange and correlation functionals. European Physical Journal B, 2018, 91, 1.	1.5	2
14	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
15	Optimal control with nonadiabatic molecular dynamics: Application to the Coulomb explosion of sodium clusters. Physical Review A, 2016, 94, .	2.5	2
16	Tailored pump-probe transient spectroscopy with time-dependent density-functional theory: controlling absorption spectra. European Physical Journal B, 2016, 89, 1.	1.5	17
17	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
18	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

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19	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
20	Nonextensive thermodynamic functions in the SchrÃ¶dinger-Gibbs ensemble. Physical Review E, 2015, 91, 022137.	2.1	2
21	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
22	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
23	Optimal control of high-harmonic generation by intense few-cycle pulses. Physical Review A, 2014, 90, .	2.5	20
24	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
25	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
26	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
27	Water molecules in ultrashort intense laser fields. Chemical Physics, 2013, 414, 45-52.	1.9	36
28	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
29	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
30	Time-dependent density-functional theory in massively parallel computer architectures: the octopus project. Journal of Physics Condensed Matter, 2012, 24, 233202.	1.8	181
31	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
32	Quantum Optimal Control. Lecture Notes in Physics, 2012, , 265-276.	0.7	2
33	On the Combination of TDDFT with Molecular Dynamics: New Developments. Lecture Notes in Physics, 2012, , 301-315.	0.7	3
34	Statistics and NosÃ© formalism for Ehrenfest dynamics. Journal of Physics A: Mathematical and Theoretical, 2011, 44, 395004.	2.1	26
35	Optimization schemes for selective molecular cleavage with tailored ultrashort laser pulses. Chemical Physics, 2011, 391, 50-61.	1.9	28
36	Quantum optimal control theory in the linear response formalism. Physical Review A, 2011, 84, .	2.5	10

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37	Optimal control of the electronic current density: Application to one- and two-dimensional one-electron systems. Physical Review A, 2011, 83, .	2.5	6
38	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>CO</mml:mi>	7.8	152
39	Ab initiomolecular dynamics on the electronic Boltzmann equilibrium distribution. New Journal of Physics, 2010, 12, 083064.	2.9	11
40	Acceleration of quantum optimal control theory algorithms with mixing strategies. Physical Review E, 2009, 79, 056704.	2.1	10
41	Exact Coulomb cutoff technique for supercell calculations in two dimensions. Physical Review B, 2009, 80, .	3.2	13
42	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
43	Modified Ehrenfest Formalism for Efficient Large-Scale ab initio Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 728-742.	5.3	124
44	Femtosecond laser pulse shaping for enhanced ionization. Europhysics Letters, 2009, 87, 53001.	2.0	34
45	Optical and magnetic properties of boron fullerenes. Physical Chemistry Chemical Physics, 2009, 11, 4523.	2.8	50
46	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
47	Coherent quantum switch driven by optimized laser pulses. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 1593-1595.	2.7	6
48	Electron localization function for two-dimensional systems. Physical Review B, 2008, 77, .	3.2	16
49	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
50	Optimal laser control of double quantum dots. Physical Review B, 2008, 77, .	3.2	32
51	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
52	Cluster-surface and cluster-cluster interactions:Ab initiocalculations and modeling of asymptotic van der Waals forces. Physical Review B, 2008, 78, .	3.2	26
53	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
54	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

#	Article	IF	Citations
55	Optimal Control of Quantum Rings by Terahertz Laser Pulses. Physical Review Letters, 2007, 98, 157404.	7.8	102
56	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
57	Molecules and clusters in strong laser fields. , 2007, , 485-617.		3
58	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
59	Photoabsorption spectra of Ti8C12 metallocarbohedrynes: Theoretical spectroscopy within time-dependent density functional theory. Journal of Chemical Physics, 2006, 125, 074311.	3.0	16
60	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
61	Optical Absorption of the Blue Fluorescent Protein: A First-Principles Study. Journal of the American Chemical Society, 2005, 127, 12329-12337.	13.7	69
62	Excited states dynamics in time-dependent density functional theory. European Physical Journal D, 2004, 28, 211-218.	1.3	126
63	Calculation of the optical spectrum of the Ti8C12 and V8C12 Met-Cars. Chemical Physics Letters, 2004, 398, 292-296.	2.6	12
64	Propagators for the time-dependent Kohnâ€“Sham equations. Journal of Chemical Physics, 2004, 121, 3425-3433.	3.0	477
65	Optical Properties of Nanostructures from Time-Dependent Density Functional Theory. Journal of Computational and Theoretical Nanoscience, 2004, 1, 231-255.	0.4	21
66	octopus: a first-principles tool for excited electronâ€“ion dynamics. Computer Physics Communications, 2003, 151, 60-78.	7.5	671
67	A Tutorial on Density Functional Theory. Lecture Notes in Physics, 2003, , 218-256.	0.7	40
68	Time-Dependent Density-Functional Approach for Biological Chromophores: The Case of the Green Fluorescent Protein. Physical Review Letters, 2003, 90, 258101.	7.8	181
69	Solution of Poisson's equation for finite systems using plane-wave methods. Canadian Journal of Physics, 2003, 81, 1151-1164.	1.1	39
70	Can optical spectroscopy directly elucidate the ground state of C20?. Journal of Chemical Physics, 2002, 116, 1930-1933.	3.0	55
71	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
72	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