Frederico V Prudente

List of Publications by Year
in descending order

75	1,050	516710 16	454955 30
papers	citations	h-index	g-index

77	77	77	685
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Thermodynamic Signatures of Structural Transitions and Dissociation of Charged Colloidal Clusters: A Parallel Tempering Monte Carlo Study. Molecules, 2022, 27, 2581.	3.8	2
2	Intermolecular Forces: From Atoms and Molecules to Nanostructures. Molecules, 2022, 27, 3072.	3.8	3
3	Modeling microsolvation clusters with electronic-structure calculations guided by analytical potentials and predictive machine learning techniques. Physical Chemistry Chemical Physics, 2021, 23, 1738-1749.	2.8	10
4	Evaluating Bohmâ€™s quantum force in the scattering process by a classical potential. European Journal of Physics, 2021, 42, 025406.	0.6	1
5	On the stabilization of the Li$$^+$$-Li$$^+$$ interaction by microsolvation with rare-gas atoms. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	1
6	On the oscillating properties of a two-electron quantum dot in the presence of a magnetic field. Journal of Physics B: Atomic, Molecular and Optical Physics, 2021, 54, 11LT01.	1.5	3
7	Coulomb correlation and information entropies in confined helium-like atoms. European Physical Journal D, 2021, 75, 1.	1.3	7
8	A variational R-matrix finite element procedure for solving ultra-cold collision problems. Computational and Applied Mathematics, 2021, 40, 1.	2.2	1
9	Information and quantum theories: an analysis in one-dimensional systems. European Journal of Physics, 2020, 41, 025405.	0.6	7
10	Cross Sections and Asymmetry Parameters for Formic Acid in the Vacuum-Ultraviolet Energy Range. Journal of Physical Chemistry A, 2020, 124, 6478-6485.	2.5	2
11	Oscillating properties of a two-electron quantum dot in the presence of a magnetic field. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 185001.	1.5	8
12	A thermodynamic view on the microsolvation of ions by rare gas: application to Li⁺ with argon. Physical Chemistry Chemical Physics, 2020, 22, 10882-10892.	2.8	8
13	Exploring the firstâ€shell and secondâ€shell structures arising in the microsolvation of Li⁺ by rare gases. International Journal of Quantum Chemistry, 2019, 119, e25860.	2.0	9
14	Photoabsorption and Photoionization Cross Sections of Pyridine in the Vacuum-Ultraviolet Energy Range. Journal of Physical Chemistry A, 2019, 123, 5164-5170.	2.5	3
15	Effect of a laser field in the confinement potential of two electrons in a double quantum dot. Journal of Physics B: Atomic, Molecular and Optical Physics, 2019, 52, 095103.	1.5	5
16	Microsolvation of Li⁺ in a Mixture of Argon and Krypton: Unveiling the Most Stable Structures of the Clusters. Journal of Physical Chemistry A, 2019, 123, 2867-2873.	2.5	9
17	Shannon entropy: A study of confined hydrogenic-like atoms. Chemical Physics Letters, 2018, 691, 401-407.	2.6	36
18	Quantum angular momentum, projective geometry and the networks of seven and ten spins: Fano, Desargues and alternative incidence configurations. Journal of Molecular Spectroscopy, 2017, 337, 153-162.	1.2	6

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19	Couplings and recouplings of four angular momenta: Alternative 9j symbols and spin addition diagrams. Journal of Molecular Modeling, 2017, 23, 147.	1.8	8
20	Photoabsorption and photoionization cross sections for formaldehyde in the vacuum-ultraviolet energy range. Journal of Chemical Physics, 2017, 146, .	3.0	11
21	Solvation of Li⁺ by argon: how important are three-body forces?. Physical Chemistry Chemical Physics, 2017, 19, 25707-25716.	2.8	13
22	Communication: Protonation process of formic acid from the ionization and fragmentation of dimers induced by synchrotron radiation in the valence region. Journal of Chemical Physics, 2016, 144, 141101.	3.0	7
23	Ionization and Fragmentation of DCOOD Induced by Synchrotron Radiation at the Oxygen 1s Edge: The Role of Dimer Formation. Journal of Physical Chemistry A, 2016, 120, 5325-5336.	2.5	5
24	Choice of atomic basis set for the study of two electrons in a harmonic anisotropic quantum dot using a configuration interaction approach. Journal of Physics B: Atomic, Molecular and Optical Physics, 2016, 49, 145004.	1.5	5
25	Umbrella motion of the methyl cation, radical, and anion molecules. European Physical Journal D, 2016, 70, 1.	1.3	4
26	Umbrella motion of the methyl cation, radical, and anion molecules. European Physical Journal D, 2016, 70, 1.	1.3	1
27	STUDY OF SHANNON ENTROPY IN THE CONTEXT OF QUANTUM MECHANICS: AN APPLICATION TO FREE AND CONFINED HARMONIC OSCILLATOR. Quimica Nova, 2016, , .	0.3	3
28	A quantum Monte Carlo study of confined quantum systems: application to harmonic oscillator and hydrogenic-like atoms. Journal of Physics B: Atomic, Molecular and Optical Physics, 2015, 48, 055002.	1.5	11
29	Ionization and Fragmentation of Formamide Induced by Synchrotron Radiation in the Valence Region via Photoelectron Photoion Coincidence Measurements and Density Functional Theory Calculations. Journal of Physical Chemistry A, 2015, 119, 10300-10308.	2.5	8
30	Angular Momentum Coupling and Discrete Quantum Mechanics: the 10-Spin Network, the Pentagonal Relationship, an Eigenvalue Equation and Semiclassical Limits. Revista Processos QuÃmicos, 2015, 9, 209-212.	0.0	0
31	Photostability studies of prebiotic molecules at the VUV region. Journal of Physics: Conference Series, 2014, 488, 022035.	0.4	0
32	Confined Quantum Systems Using the Finite Element and Discrete Variable Representation Methods. , 2014, , 101-143.		3
33	Pekeris approximation â€“ another perspective. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 3027-3032.	2.1	21
34	Alternative hyperspherical adiabatic decoupling scheme for tetratomic molecules: quantum two-dimensional study of the ammonia umbrella motion. European Physical Journal D, 2013, 67, 1.	1.3	5
35	Roto-torsional Levels for Symmetric and Asymmetric Systems: Application to HOOH and HOOD Systems. Lecture Notes in Computer Science, 2013, , 1-16.	1.3	2
36	Message from the QMCSA 2012 Chairs. , 2012, , .		0

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37	Message from the Local Organizing Committee Chair. , 2012, , .		0
38	Theoreticalâ€“Experimental Study of Formic Acid Photofragmentation in the Valence Region. Journal of Physical Chemistry A, 2012, 116, 6693-6701.	2.5	7
39	Study of Plasma Effect on Spectral Properties of Hydrogenic and Helium-Like Ions Using the Finite Element Method. , 2012, , .		2
40	Direct fit of spectroscopic data of diatomic molecules by using genetic algorithms: II. The ground state of RbCs. Journal of Physics B: Atomic, Molecular and Optical Physics, 2011, 44, 225102.	1.5	7
41	A study of the electron structure of endohedrally confined atoms using a model potential. Journal of Physics B: Atomic, Molecular and Optical Physics, 2011, 44, 015003.	1.5	68
42	A variational adiabatic hyperspherical finite element R matrix methodology: general formalism and application to HÂ+ÂH2 reaction. European Physical Journal D, 2011, 64, 287-296.	1.3	5
43	Analysis of vibrational modes of the P₄ molecule through hyperspherical variants of the local orthogonal coordinates: The limit of dissociation in dimers. International Journal of Quantum Chemistry, 2011, 111, 1719-1733.	2.0	5
44	Time-dependent wave packet calculation of the LiH + H reactive scattering on a new potential energy surface. Chemical Physics Letters, 2009, 474, 18-22.	2.6	35
45	Intramolecular Dynamics of RSâ˜SRâ€² Systems (R, Râ€² = H, F, Cl, CH3, C2 H5): Torsional Potentials, Energy Levels, Partition Functions. Journal of Physical Chemistry A, 2009, 113, 3804-3813.	2.5	29
46	A new genetic algorithm to be used in the direct fit of potential energy curves toab initioand spectroscopic data. Journal of Physics B: Atomic, Molecular and Optical Physics, 2008, 41, 085103.	1.5	38
47	Level distributions, partition functions, and rates of chirality changing processes for the torsional mode around Oâ€“O bonds. Journal of Chemical Physics, 2008, 129, 154316.	3.0	34
48	The characteristic function method applied to molecular dynamics of inelastic granular gases. Physica A: Statistical Mechanics and Its Applications, 2007, 373, 392-416.	2.6	1
49	Diabatic potential-optimized discrete variable representation: application to photodissociation process of the CO molecule. Journal of Physics B: Atomic, Molecular and Optical Physics, 2007, 40, 2075-2090.	1.5	4
50	Theoretical calculations of the structure and UVâ€“vis absorption spectra of hydrated C60 fullerene. Carbon, 2006, 44, 2925-2930.	10.3	35
51	The multiple dependence of the velocity distributions of granular gases on the simulation conditions. Physica A: Statistical Mechanics and Its Applications, 2006, 371, 50-53.	2.6	1
52	Sobre o confinamento espacial de sistemas quÃ¢nticos: o oscilador harmÃ´nico unidimensional e o Ã¡tomo de hidrogÃªnio. Revista Brasileira De Ensino De Fisica, 2005, 27, 395-405.	0.2	6
53	A study of the confined hydrogen atom using the finite element method. Journal of Physics B: Atomic, Molecular and Optical Physics, 2005, 38, 2811-2825.	1.5	56
54	A study of two-electron quantum dot spectrum using discrete variable representation method. Journal of Chemical Physics, 2005, 123, 224701.	3.0	35

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55	The fitting of potential energy and transition moment functions using neural networks: transition probabilities in OH (A2Î£+â†'X2Î). Chemical Physics, 2004, 297, 153-161.	1.9	30
56	Guiding Function and Basis Function Optimization in Correlation Function Quantum Monte Carlo Calculations of Vibrational Excited States in Molecules. Journal of Physical Chemistry A, 2004, 108, 1305-1311.	2.5	1
57	Time dependent wave packet study of the electronically non-adiabatic Clâ€‰+â€‰H2reaction using a one-dimensional model. Physical Chemistry Chemical Physics, 2003, 5, 2354-2359.	2.8	4
58	A Direct Evaluation of the Partition Function and Thermodynamic Data for Water at High Temperatures. Journal of Physical Chemistry A, 2002, 106, 6193-6200.	2.5	10
59	Vibrational partition functions for atomÃ¢â‚¬â€œdiatom and atomÃ¢â‚¬â€œtriatom van der Waals systems. Physical Chemistry Chemical Physics, 2001, 3, 5000-5005.	2.8	7
60	On the Rovibrational Partition Function of Molecular Hydrogen at High Temperatures. Journal of Physical Chemistry A, 2001, 105, 9518-9521.	2.5	22
61	Calculation of the Rovibrational Partition Function Using Classical Methods with Quantum Corrections. Journal of Physical Chemistry A, 2001, 105, 5272-5279.	2.5	14
62	Quantum Monte Carlo study of vibrational states of silanone. Chemical Physics Letters, 2000, 321, 121-125.	2.6	7
63	Correlation function quantum Monte Carlo studies of rovibrational excited states in molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, R285-R313.	1.5	16
64	Evaluation of vibrational partition functions for polyatomic systems: quantum versus classical methods for H2O and ArÂ·Â·Â·CN. Physical Chemistry Chemical Physics, 2000, 2, 4121-4129.	2.8	14
65	Generalized rotating wave function for quantum Monte Carlo calculations of rovibrational levels ofn-body systems. Physical Review A, 1999, 61, .	2.5	5
66	A study of confined quantum systems using the Woods-Saxon potential. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 2461-2470.	1.5	66
67	Quantum-Monte Carlo study of rovibrational states of molecular systems. Chemical Physics Letters, 1999, 302, 249-254.	2.6	16
68	Optimized mesh for the finite-element method using a quantum-mechanical procedure. Chemical Physics Letters, 1999, 302, 43-48.	2.6	17
69	Quantum scattering using a novel implementation based on the variational R matrix formalism and the finite element method: a comparative study. Chemical Physics Letters, 1999, 309, 471-478.	2.6	9
70	Quantum Monte Carlo study of rovibrational states utilizing rotating wavefunctions: Application to H2O. Journal of Chemical Physics, 1999, 111, 6311-6315.	3.0	14
71	The fitting of potential energy surfaces using neural networks. Application to the study of the photodissociation processes. Chemical Physics Letters, 1998, 287, 585-589.	2.6	57
72	The fitting of potential energy surfaces using neural networks: Application to the study of vibrational levels of H3+. Journal of Chemical Physics, 1998, 109, 8801-8808.	3.0	108

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73	Discrete variable representation and negative imaginary potential to study metastable states and photodissociation processes. Application to diatomic and triatomic molecules. Computational and Theoretical Chemistry, 1997, 394, 169-180.	1.5	13
74	A novel finite element method implementation for calculating bound states of triatomic systems: Application to the water molecule. Theoretica Chimica Acta, 1994, 89, 415-427.	0.8	16
75	O mÃ©todo do elemento finito aplicado ao estudo de colisÃµes atÃ´micas e moleculares. , 0, , .		0