

# Frederico V Prudente

## List of Publications by Year in descending order

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75  
papers

1,050  
citations

516710

16  
h-index

454955

30  
g-index

77  
all docs

77  
docs citations

77  
times ranked

685  
citing authors

#	ARTICLE	IF	CITATIONS
1	The fitting of potential energy surfaces using neural networks: Application to the study of vibrational levels of H <sub>3</sub> <sup>+</sup> . Journal of Chemical Physics, 1998, 109, 8801-8808.	3.0	108
2	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
3	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
4	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
5	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
6	A new genetic algorithm to be used in the direct fit of potential energy curves to <i>ab initio</i> and spectroscopic data. Journal of Physics B: Atomic, Molecular and Optical Physics, 2008, 41, 085103.	1.5	38
7	Shannon entropy: A study of confined hydrogenic-like atoms. Chemical Physics Letters, 2018, 691, 401-407.	2.6	36
8	A study of two-electron quantum dot spectrum using discrete variable representation method. Journal of Chemical Physics, 2005, 123, 224701.	3.0	35
9	Theoretical calculations of the structure and UV-vis absorption spectra of hydrated C <sub>60</sub> fullerene. Carbon, 2006, 44, 2925-2930.	10.3	35
10	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
11	Level distributions, partition functions, and rates of chirality changing processes for the torsional mode around O-O bonds. Journal of Chemical Physics, 2008, 129, 154316.	3.0	34
12	The fitting of potential energy and transition moment functions using neural networks: transition probabilities in OH (A <sub>2</sub> <sup>+</sup> X <sub>2</sub> ). Chemical Physics, 2004, 297, 153-161.	1.9	30
13	Intramolecular Dynamics of RS <sup>n</sup> SR <sup>n</sup> Systems (R, R <sup>n</sup> = H, F, Cl, CH <sub>3</sub> , C <sub>2</sub> H <sub>5</sub> ): Torsional Potentials, Energy Levels, Partition Functions. Journal of Physical Chemistry A, 2009, 113, 3804-3813.	2.5	29
14	On the Rovibrational Partition Function of Molecular Hydrogen at High Temperatures. Journal of Physical Chemistry A, 2001, 105, 9518-9521.	2.5	22
15	Pekeris approximation - another perspective. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 3027-3032.	2.1	21
16	Optimized mesh for the finite-element method using a quantum-mechanical procedure. Chemical Physics Letters, 1999, 302, 43-48.	2.6	17
17	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
18	Quantum-Monte Carlo study of rovibrational states of molecular systems. Chemical Physics Letters, 1999, 302, 249-254.	2.6	16

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19	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
20	Quantum Monte Carlo study of rovibrational states utilizing rotating wavefunctions: Application to H <sub>2</sub> O. Journal of Chemical Physics, 1999, 111, 6311-6315.	3.0	14
21	Evaluation of vibrational partition functions for polyatomic systems: quantum versus classical methods for H <sub>2</sub> O and Ar·CN. Physical Chemistry Chemical Physics, 2000, 2, 4121-4129.	2.8	14
22	Calculation of the Rovibrational Partition Function Using Classical Methods with Quantum Corrections. Journal of Physical Chemistry A, 2001, 105, 5272-5279.	2.5	14
23	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
24	Solvation of Li <sup>+</sup> by argon: how important are three-body forces?. Physical Chemistry Chemical Physics, 2017, 19, 25707-25716.	2.8	13
25	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
26	Photoabsorption and photoionization cross sections for formaldehyde in the vacuum-ultraviolet energy range. Journal of Chemical Physics, 2017, 146, .	3.0	11
27	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
28	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
29	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
30	Exploring the first shell and second shell structures arising in the microsolvation of Li <sup>+</sup> by rare gases. International Journal of Quantum Chemistry, 2019, 119, e25860.	2.0	9
31	Microsolvation of Li <sup>+</sup> 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
32	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
33	Couplings and recouplings of four angular momenta: Alternative 9j symbols and spin addition diagrams. Journal of Molecular Modeling, 2017, 23, 147.	1.8	8
34	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
35	A thermodynamic view on the microsolvation of ions by rare gas: application to Li <sup>+</sup> with argon. Physical Chemistry Chemical Physics, 2020, 22, 10882-10892.	2.8	8
36	Quantum Monte Carlo study of vibrational states of silanone. Chemical Physics Letters, 2000, 321, 121-125.	2.6	7

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37	Vibrational partition functions for atom-atom and atom-atom van der Waals systems. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 5000-5005.	2.8	7
38	Direct fit of spectroscopic data of diatomic molecules by using genetic algorithms: II. The ground state of RbCs. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2011, 44, 225102.	1.5	7
39	Theoretical-Experimental Study of Formic Acid Photofragmentation in the Valence Region. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6693-6701.	2.5	7
40	Communication: Protonation process of formic acid from the ionization and fragmentation of dimers induced by synchrotron radiation in the valence region. <i>Journal of Chemical Physics</i> , 2016, 144, 141101.	3.0	7
41	Information and quantum theories: an analysis in one-dimensional systems. <i>European Journal of Physics</i> , 2020, 41, 025405.	0.6	7
42	Coulomb correlation and information entropies in confined helium-like atoms. <i>European Physical Journal D</i> , 2021, 75, 1.	1.3	7
43	Sobre o confinamento espacial de sistemas quânticos: o oscilador harmônico unidimensional e o átomo de hidrogênio. <i>Revista Brasileira De Ensino De Fisica</i> , 2005, 27, 395-405.	0.2	6
44	Quantum angular momentum, projective geometry and the networks of seven and ten spins: Fano, Desargues and alternative incidence configurations. <i>Journal of Molecular Spectroscopy</i> , 2017, 337, 153-162.	1.2	6
45	Generalized rotating wave function for quantum Monte Carlo calculations of rovibrational levels of n-body systems. <i>Physical Review A</i> , 1999, 61, .	2.5	5
46	A variational adiabatic hyperspherical finite element R matrix methodology: general formalism and application to $\text{H}^+\text{H}_2$ reaction. <i>European Physical Journal D</i> , 2011, 64, 287-296.	1.3	5
47	Analysis of vibrational modes of the $\text{P}_4$ molecule through hyperspherical variants of the local orthogonal coordinates: The limit of dissociation in dimers. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1719-1733.	2.0	5
48	Alternative hyperspherical adiabatic decoupling scheme for tetratomic molecules: quantum two-dimensional study of the ammonia umbrella motion. <i>European Physical Journal D</i> , 2013, 67, 1.	1.3	5
49	Ionization and Fragmentation of DCOOD Induced by Synchrotron Radiation at the Oxygen 1s Edge: The Role of Dimer Formation. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5325-5336.	2.5	5
50	Choice of atomic basis set for the study of two electrons in a harmonic anisotropic quantum dot using a configuration interaction approach. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2016, 49, 145004.	1.5	5
51	Effect of a laser field in the confinement potential of two electrons in a double quantum dot. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2019, 52, 095103.	1.5	5
52	Time dependent wave packet study of the electronically non-adiabatic $\text{Cl} + \text{H}_2$ reaction using a one-dimensional model. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 2354-2359.	2.8	4
53	Diabatic potential-optimized discrete variable representation: application to photodissociation process of the CO molecule. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2007, 40, 2075-2090.	1.5	4
54	Umbrella motion of the methyl cation, radical, and anion molecules. <i>European Physical Journal D</i> , 2016, 70, 1.	1.3	4

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55	Photoabsorption and Photoionization Cross Sections of Pyridine in the Vacuum-Ultraviolet Energy Range. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5164-5170.	2.5	3
56	On the oscillating properties of a two-electron quantum dot in the presence of a magnetic field. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2021, 54, 11LT01.	1.5	3
57	Confined Quantum Systems Using the Finite Element and Discrete Variable Representation Methods. , 2014, , 101-143.		3
58	STUDY OF SHANNON ENTROPY IN THE CONTEXT OF QUANTUM MECHANICS: AN APPLICATION TO FREE AND CONFINED HARMONIC OSCILLATOR. <i>Quimica Nova</i> , 2016, , .	0.3	3
59	Intermolecular Forces: From Atoms and Molecules to Nanostructures. <i>Molecules</i> , 2022, 27, 3072.	3.8	3
60	Study of Plasma Effect on Spectral Properties of Hydrogenic and Helium-Like Ions Using the Finite Element Method. , 2012, , .		2
61	Cross Sections and Asymmetry Parameters for Formic Acid in the Vacuum-Ultraviolet Energy Range. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6478-6485.	2.5	2
62	Rototorsional Levels for Symmetric and Asymmetric Systems: Application to HOOH and HOOD Systems. <i>Lecture Notes in Computer Science</i> , 2013, , 1-16.	1.3	2
63	Thermodynamic Signatures of Structural Transitions and Dissociation of Charged Colloidal Clusters: A Parallel Tempering Monte Carlo Study. <i>Molecules</i> , 2022, 27, 2581.	3.8	2
64	Guiding Function and Basis Function Optimization in Correlation Function Quantum Monte Carlo Calculations of Vibrational Excited States in Molecules. <i>Journal of Physical Chemistry A</i> , 2004, 108, 1305-1311.	2.5	1
65	The multiple dependence of the velocity distributions of granular gases on the simulation conditions. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2006, 371, 50-53.	2.6	1
66	The characteristic function method applied to molecular dynamics of inelastic granular gases. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2007, 373, 392-416.	2.6	1
67	Umbrella motion of the methyl cation, radical, and anion molecules. <i>European Physical Journal D</i> , 2016, 70, 1.	1.3	1
68	Evaluating Bohm's quantum force in the scattering process by a classical potential. <i>European Journal of Physics</i> , 2021, 42, 025406.	0.6	1
69	On the stabilization of the $\text{Li}^+ \cdots \text{Li}^+$ interaction by microsolvation with rare-gas atoms. <i>Theoretical Chemistry Accounts</i> , 2021, 140, 1.	1.4	1
70	A variational R-matrix finite element procedure for solving ultra-cold collision problems. <i>Computational and Applied Mathematics</i> , 2021, 40, 1.	2.2	1
71	Message from the QMCSA 2012 Chairs. , 2012, , .		0
72	Message from the Local Organizing Committee Chair. , 2012, , .		0

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73	Photostability studies of prebiotic molecules at the VUV region. Journal of Physics: Conference Series, 2014, 488, 022035.	0.4	0
74	Angular Momentum Coupling and Discrete Quantum Mechanics: the 10-Spin Network, the Pentagonal Relationship, an Eigenvalue Equation and Semiclassical Limits. Revista Processos Químicos, 2015, 9, 209-212.	0.0	0
75	O método do elemento finito aplicado ao estudo de colisões atômicas e moleculares. , 0, , .		0