Joao Pedro Braga

List of Publications by Year
in descending order

114	746	623734	839539
papers	citations	14 h-index	18 g-index

116	116	116	497
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	SVM-KM: speeding SVMs learning with a priori cluster selection and k-means. , 0, , .		74
2	Competition between kinetic models in thermal decomposition: analysis by artificial neural network. Thermochimica Acta, 2004, 412, 107-111.	2.7	29
3	Diffusion coefficient distribution from NMR-DOSY experiments using Hopfield neural network. Journal of Magnetic Resonance, 2006, 182, 22-28.	2.1	27
4	Quantum second virial coefficient calculation for the 4He dimer on a recent potential. Journal of the Brazilian Chemical Society, 2013, 24, 363-368.	0.6	24
5	Electronic Quenching of N(²D) by N₂: Theoretical Predictions, Comparison with Experimental Rate Constants, and Impact on Atmospheric Modeling. Journal of Physical Chemistry Letters, 2013, 4, 2292-2297.	4.6	22
6	Unified description of chemical bonding in H2 isotopomers, including Ps2, Î¼2 and bi-excitons. Chemical Physics Letters, 2000, 332, 139-144.	2.6	21
7	Artificial neural network applied to solid state thermal decomposition. Journal of Thermal Analysis and Calorimetry, 2003, 74, 811-818.	3.6	20
8	Size evolution of structures and energetics of iron clusters (Fen, nâ‰36): Molecular dynamics studies using a Lennardâ€"Jones type potential. Journal of Alloys and Compounds, 2005, 403, 349-356.	5.5	20
9	Solving ill-posed problems faster using fractional-order Hopfield neural network. Journal of Computational and Applied Mathematics, 2021, 381, 112984.	2.0	20
10	Complete CI calculations on the ground state of HeH. Chemical Physics Letters, 1984, 110, 40-42.	2.6	16
11	Hopfield neural network model for calculating the potential energy function from second virial data. Chemical Physics, 2000, 260, 347-352.	1.9	16
12	Electronic Quenching in N(²D) + N₂ Collisions: A State-Specific Analysis via Surface Hopping Dynamics. Journal of Chemical Theory and Computation, 2014, 10, 1872-1877.	5.3	16
13	Inversion of Simulated Positron Annihilation Lifetime Spectrum Using a Neural Network. Journal of Chemical Information and Computer Sciences, 2001, 41, 309-313.	2.8	15
14	Title is missing!. Journal of Mathematical Chemistry, 2001, 29, 151-161.	1.5	15
15	A theoretical study of the non-adiabatic charge transfer process Ar2+(3P) + He(1S) â†' Ar+(2P) + He+(2S). Molecular Physics, 1986, 57, 665-674.	1.7	14
16	Rate constants and absorption coefficients from experimental data: An inversion procedure based on recursive neural networks. Chemometrics and Intelligent Laboratory Systems, 2009, 96, 84-87.	3.5	14
17	Spherical potential energy function from second virial coefficient using Tikhonov regularization and truncated singular value decomposition. Chemical Physics Letters, 1998, 296, 233-238.	2.6	13
18	Accurate Explicit-Correlation-MRCI-Based DMBE Potential-Energy Surface for Ground-State CNO. Journal of Physical Chemistry A, 2018, 122, 4198-4207.	2.5	13

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19	Nonlinear global inversion of potential energy surfaces from the experimentally determined second virial coefficients. Chemical Physics Letters, 2003, 378, 406-409.	2.6	12
20	Retrieval of transverse relaxation time distribution from spin-echo data by recurrent neural network. Journal of Magnetic Resonance, 2005, 177, 146-151.	2.1	12
21	Dataset structure as prior information for parameter-free regularization of extreme learning machines. Neurocomputing, 2015, 169, 288-294.	5.9	12
22	Artificial neural network applied for predicting rainbow trajectories in atomic and molecular classical collisions. Journal of Chemical Physics, 1997, 107, 9954-9959.	3.0	11
23	A general algorithm to solve linear and nonlinear inverse problems. Journal of the Brazilian Chemical Society, 2007, 18, 1342-1347.	0.6	11
24	Potential energy function from differential crossâ€section data: An inverse quantum scattering theory approach. International Journal of Quantum Chemistry, 2008, 108, 2623-2627.	2.0	11
25	A generalized Mittag-Leffler function to describe nonexponential chemical effects. Applied Mathematical Modelling, 2016, 40, 7971-7976.	4.2	11
26	Structures and energetics of CO2â€“Arn clusters (nâ€‚=â€‚1â€“21) based on a non-rigid potential model. Canadian Journal of Chemistry, 2007, 85, 47-55.	1.1	10
27	A comparison of classical and quantal transition probabilities for a non-adiabatic atom-atom collision. Chemical Physics Letters, 1985, 120, 147-150.	2.6	9
28	Quantum and classical two-dimensional analysis of rainbow structures in the Xe+CO2rotational excitation at 0.2 eV collision energy and on a repulsive potential. Physical Review A, 1995, 52, 342-349.	2.5	9
29	Force field inverse problems using recurrent neural networks. Chemical Physics Letters, 2006, 423, 357-360.	2.6	9
30	Vibrational energy transfer in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si20.gif" overflow="scroll"><mml:mrow><mml:mi mathvariant="normal">N</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:msup><mml:mrow) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.6	9
31	mathvariant="normal">N</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml: A genetic algorithm survey on closed-shell atomic nitrogen clusters employing a quantum chemical approach. Journal of Molecular Modeling, 2018, 24, 196.	1.8	9
32	Analysis of state-to-state differential cross sections in two-dimensional Xe-CO2scattering with long-range effects. Physical Review A, 1996, 54, 2091-2098.	2.5	8
33	Long-range spherical potential energy function from the second virial coefficient using decomposition into subspaces. Physical Chemistry Chemical Physics, 2001, 3, 4355-4358.	2.8	8
34	Neural network in the inverse problem of liquid argon structure factor: from gas-to-liquid radial distribution function. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	8
35	The bound, metastable and virtual states of rare gas hydrides. Molecular Physics, 1984, 53, 295-299.	1.7	7
36	Radial basis function networks for obtaining long range dispersion coefficients from second virial data. Physical Chemistry Chemical Physics, 2000, 2, 103-107.	2.8	7

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37	Phonon density of states from the experimental heat capacity: an improved distribution function for solid aluminium using an inverse framework. Journal of Molecular Modeling, 2014, 20, 2360.	1.8	7
38	Quasiclassical Study of the C(³P) + NO(X²Î) and O(³P) + CN(X²Î£⁺) Collisional Processes on an Accurate DMBE Potential Energy Surface. Journal of Physical Chemistry A, 2019, 123, 7195-7200.	2.5	7
39	Improving a Tikhonov regularization method with a fractional-order differential operator for the inverse black body radiation problem. Inverse Problems in Science and Engineering, 2020, 28, 1513-1527.	1.2	7
40	A comparison of state-to-state rotational total cross sections using two- and three-dimensional close coupled approaches. Chemical Physics Letters, 1996, 251, 346-352.	2.6	6
41	Potential energy function from second virial data using sensitivity analysis. Inverse Problems in Science and Engineering, 2006, 14, 581-587.	1.2	6
42	A kinetic study of jack-bean urease denaturation by a new dithiocarbamate bismuth compound. Chemical Physics Letters, 2012, 548, 85-89.	2.6	6
43	Variable phase equation in quantum scattering. Revista Brasileira De Ensino De Fisica, 2014, 36, .	0.2	6
44	DFT Study of Small Gold Clusters, Au n (2â‰ n â‰ 6): Stability and Charge Distribution Using M08-SO Functional. Brazilian Journal of Physics, 2018, 48, 390-397.	1.4	6
45	Thermodynamic consistency by a modified Perkusâ€“Yevick theory using the Mittag-Leffler function. Physica A: Statistical Mechanics and Its Applications, 2021, 576, 126065.	2.6	6
46	Probability density function from experimental positron annihilation lifetime spectra. Journal of the Brazilian Chemical Society, 2005, 16, 93-97.	0.6	6
47	The rate of convergence of the S matrix for the renormalized Numerov and log-derivative methods. Journal of Computational Chemistry, 1989, 10, 413-416.	3.3	5
48	Coriolis coupling on the rotational and vibrational energy transfer in H2O+ Ar collisions: Classical trajectories simulation. International Journal of Quantum Chemistry, 2006, 106, 2643-2649.	2.0	5
49	Macromolecular properties from light-scattering experimental data using linear inverse problem theory. International Journal of Quantum Chemistry, 2006, 106, 2731-2736.	2.0	5
50	Structures and energies of Ar_nH₂O (n = 1â€“26) clusters using a nonrigid potential surface: A molecular dynamics simulation. International Journal of Quantum Chemistry, 2008, 108, 2523-2529.	2.0	5
51	Radial distribution function for liquid gallium from experimental structure factor: a Hopfield neural network approach. Journal of Molecular Modeling, 2020, 26, 193.	1.8	5
52	Quantum and semiclassical analysis of spin-change cross sections for the alkali diatomic molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 1990, 23, 3113-3122.	1.5	4
53	A critical analysis of the two-dimensional atom ellipsoid model to study rotational collisions. Chemical Physics, 1996, 213, 303-311.	1.9	4
54	Recurrent Neural Network Model to Retrieve the Long Range Spherical Potential Energy Function from Second Virial Coefficient. Inverse Problems in Science and Engineering, 2002, 10, 153-162.	0.5	4

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55	Uso de redes neurais recorrentes na determinaÃ§Ã£o das constantes de acidez para a 7-epiclusianona em misturas etanol-Ã¡gua. Quimica Nova, 2012, 35, 91-96.	0.3	4
56	Indirect Solution of Ornstein-Zernike Equation Using the Hopfield Neural Network Method. Brazilian Journal of Physics, 2020, 50, 489-494.	1.4	4
57	Hopfield Neural Network-Based Algorithm Applied to Differential Scanning Calorimetry Data for Kinetic Studies in Polymorphic Conversion. Journal of the Brazilian Chemical Society, 0, , .	0.6	4
58	Partial radial distribution functions for a two-component glassy solid, GeSe$$_{3}$$, from scattering experimental data using an artificial intelligence framework. Journal of Molecular Modeling, 2022, 28, 99.	1.8	4
59	A comparative study of quantum mechanical and classical trajectory calculations for anA+BCcollinear non-adiabatic collision. Molecular Physics, 1988, 65, 909-923.	1.7	3
60	Analysis of state-to-state classical rotational cross-sections for Arâ€“CO2 collisions. Physical Chemistry Chemical Physics, 1999, 1, 23-27.	2.8	3
61	ReflexÃµes sobre a contribuiÃ§Ã£o da Carnot Ã primeira lei da termodinÃ¢mica. Quimica Nova, 2004, 27, 513-515.	0.3	3
62	Coriolis coupling effects on energy transfer: classical-trajectories analysis for CO2 + Ar collisions. Canadian Journal of Chemistry, 2007, 85, 983-988.	1.1	3
63	Cusp conditions for two electrons atoms in the Hylleraas aproximation. Journal of Physics B: Atomic, Molecular and Optical Physics, 2018, 51, 135001.	1.5	3
64	Accurate DMBE potential-energy surface for CNO(2Aâ€³) and rate coefficients in C(3P)+NO collisions. Journal of Chemical Physics, 2021, 154, 034303.	3.0	3
65	Coordenadas cartesianas moleculares a partir da geometria dos modos normais de vibraÃ§Ã£o. Quimica Nova, 2007, 30, 497-500.	0.3	3
66	A route to inversion for rotational collisions using hard shape potentials. Chemical Physics, 1996, 205, 401-406.	1.9	2
67	An analysis of rotational transition probabilities and cross sections using close coupling, hard shape, and classical trajectory methods. Journal of Chemical Physics, 1996, 105, 5792-5797.	3.0	2
68	Two-dimensional atom ellipsoid model for analysing Heâ€“Li2[(A)1Î£u+] rotational collisions with multiple impacts. Physical Chemistry Chemical Physics, 2001, 3, 5521-5527.	2.8	2
69	Applications of genetic algorithms for inverting positron lifetime spectrum. Chemical Physics Letters, 2005, 412, 353-358.	2.6	2
70	Comparative analysis of ArnCl2 (2 â‰¤n â‰¤ 30) clusters taking into account molecular relaxation effects. International Journal of Quantum Chemistry, 2006, 106, 2752-2762.	2.0	2
71	Ion-polymer interaction analysis: an inversion of NMR spin echo experimental data. Brazilian Journal of Physics, 2010, 40, .	1.4	2
72	Methane combustion kinetic rate constants determination: an ill-posed inverse problem analysis. Quimica Nova, 2013, 36, 262-266.	0.3	2

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73	Potential energy function information from quantum phase shift using the variable phase method. Journal of Molecular Modeling, 2014, 20, 2317.	1.8	2
74	Accurate multi-reference study of Si3 electronic manifold. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	2
75	Accurate potential energy curve for helium dimer retrieved from viscosity coefficient data at very low temperatures. Physica A: Statistical Mechanics and Its Applications, 2017, 487, 32-39.	2.6	2
76	Fractional kinetics on thermal analysis: application to lumefantrine thermal decomposition. Journal of Molecular Modeling, 2020, 26, 170.	1.8	2
77	TRANSMISSION AND REFLECTION COEFFICIENTS BY THE VARIABLE AMPLITUDE METHOD. Quimica Nova, 2016, , .	0.3	2
78	Normalization of the Fox?Goodwin algorithm to calculate scattering matrices in an adiabatic basis at low and high collision energies. Journal of Computational Chemistry, 1996, 17, 1559-1563.	3.3	1
79	State-to-state quantum three-dimensional rotational total cross sections from two-dimensional close-coupled equations. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 1723-1730.	1.5	1
80	Classical trajectory study on Arâ^'Cl2 van der Waals system using a recent potential. Chemical Physics, 1999, 241, 305-311.	1.9	1
81	Colapso da equipartiÃ§Ã£o da energia. Quimica Nova, 2001, 24, 693-699.	0.3	1
82	TRAINING SVMs WITH EDR ALGORITHM. International Journal of Neural Systems, 2001, 11, 257-263.	5.2	1
83	A molecular dynamics simulation of ArnO3 (n=1â€“21) van der Waals complexes: Size evolution of stable structures. Chemical Physics Letters, 2009, 472, 194-199.	2.6	1
84	O efeito de Coriolis: de pÃªndulos a molÃ©culas. Quimica Nova, 2010, 33, 1416-1420.	0.3	1
85	CÃ¡lculo do volume na equaÃ§Ã£o de van der Waals pelo mÃ©todo de cardano. Quimica Nova, 2010, 33, 1325-1329.	0.3	1
86	Retrieval of kinetic rates in reactions with semi batch liquid phase using ill-posed inverse problem theory. Quimica Nova, 2011, 34, 213-217.	0.3	1
87	Functional sensitivity analysis approach to retrieve the potential energy function from the quantum second virial coefficient. Physica A: Statistical Mechanics and Its Applications, 2019, 536, 122539.	2.6	1
88	Electronic Entropy as a Periodic Property of the Elements: A Theoretical Chemistry Approach. Journal of Chemical Education, 2021, 98, 2574-2577.	2.3	1
89	Radial Distribution Function for a Hard Sphere Liquid: A Modified Percus-Yevick and Hypernetted-Chain Closure Relations. Journal of the Brazilian Chemical Society, 0, , .	0.6	1
90	THE HYLLERAAS METHOD FOR TWO ELECTRONS ATOMS. Quimica Nova, 0, , .	0.3	1

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91	ILL-POSED INVERSE PROBLEMS IN CHEMISTRY. Quimica Nova, 2016, , .	0.3	1
92	Parametric sensitivity analysis for the helium dimers on a model potential. Quimica Nova, 2012, 35, 910-913.	0.3	1
93	Quantum Second Virial Coefficient Calculation for the⁴He Dimer on a Recent Potential. Journal of the Brazilian Chemical Society, 2013, , .	0.6	1
94	O centenÃ¡rio da molÃ©cula de Bohr. Quimica Nova, 2013, 36, 1078-1082.	0.3	1
95	UMA AULA DE WALTHER NERNST NO BRASIL. Quimica Nova, 2019, , .	0.3	1
96	The symmetrization in the classical path approach applied to vibrational cross sections. Chemical Physics, 1995, 200, 137-140.	1.9	0
97	Quantum and classical path calculations of the total cross section for He+ (2S) + Ne (2p6,1S) â†' He+ (2S) + Ne (2p53s1P) with collision energy from 20 to 70.9 eV. Computational and Theoretical Chemistry, 1995, 341, 149-155.	1.5	0
98	Artificial neural networks applied to theoretical chemistry. , 0, , .		0
99	A formulaÃ§Ã£o ab-initio da segunda lei da termodinÃ¢mica. Quimica Nova, 1998, 21, 499-503.	0.3	0
100	AplicaÃ§Ã£o do modelo geomÃ©trico no estudo dos efeitos glory e rainbow em colisÃµes atÃ´micas. Quimica Nova, 1998, 21, 714-718.	0.3	0
101	Calculation of three dimensional cross-sections for the Arâ€“N2 system from two-dimensional coupled equations plus a three-dimensional boundary condition. Chemical Physics Letters, 2000, 332, 159-166.	2.6	0
102	Classical analysis of intermolecular potentials for ArÂ–CO2 rotational collisions. Canadian Journal of Chemistry, 2001, 79, 211-220.	1.1	0
103	Inversion of simulated positron annihilation lifetime spectra by moving boundary subspaces. International Journal of Quantum Chemistry, 2003, 95, 97-102.	2.0	0
104	Operador dipolo-dipolo na base de momento angular: um complemento ao estudo de ressonÃ¢ncia magnÃ©tica nuclear. Quimica Nova, 2008, 31, 1058-1061.	0.3	0
105	Hyperfine structure of 57Fe in minerals from a manganese ore deposit. Hyperfine Interactions, 2011, 203, 25-31.	0.5	0
106	From deflection function to potential energy: A Firsov approach critical analysis. International Journal of Quantum Chemistry, 2012, 112, 3141-3146.	2.0	0
107	An Illâ€posed inverse problem in enzymatic kinetics: Jackâ€Bean urease denaturation by an anionic surfactant. International Journal of Quantum Chemistry, 2012, 112, 3240-3245.	2.0	0
108	O centenÃ¡rio da Teoria de Bohr. Quimica Nova, 2013, 36, 1073-1077.	0.3	0

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109	Os cem anos do Ã¡tomo de Sommerfeld. Revista Brasileira De Ensino De Fisica, 2016, 38, .	0.2	0
110	Trailblazer: When Marie Curie went to Brazil. Nature, 2017, 551, 440-440.	27.8	0
111	Aspectos histÃ³ricos da visita de Marie Sklodowska Curie a Belo Horizonte. Quimica Nova, 2011, 34, 1888-1891.	0.3	0
112	MÃ¡xima absorÃ§Ã£o ressonante em espectroscopia MÃ¶ssbauer. Revista Brasileira De Ensino De Fisica, 2013, 35, .	0.2	0
113	Quantum Charge Transfer Study of Triply Charged Ions in the Adiabatic Representation: the (BHe)3+ System. Journal of the Brazilian Chemical Society, 1998, 9, .	0.6	0
114	Max Planckâ€™s Determination of the Avogadro Constant. Revista Brasileira De Ensino De Fisica, 0, 44, .	0.2	0