Joao Pedro Braga

List of Publications by Year
in descending order

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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	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
2	Solving ill-posed problems faster using fractional-order Hopfield neural network. Journal of Computational and Applied Mathematics, 2021, 381, 112984.	2.0	20
3	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
4	Electronic Entropy as a Periodic Property of the Elements: A Theoretical Chemistry Approach. Journal of Chemical Education, 2021, 98, 2574-2577.	2.3	1
5	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
6	Indirect Solution of Ornstein-Zernike Equation Using the Hopfield Neural Network Method. Brazilian Journal of Physics, 2020, 50, 489-494.	1.4	4
7	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
8	Fractional kinetics on thermal analysis: application to lumefantrine thermal decomposition. Journal of Molecular Modeling, 2020, 26, 170.	1.8	2
9	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
10	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
11	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
12	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
13	UMA AULA DE WALTHER NERNST NO BRASIL. Quimica Nova, 2019, , .	0.3	1
14	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
15	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
16	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
17	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
18	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

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19	Trailblazer: When Marie Curie went to Brazil. Nature, 2017, 551, 440-440.	27.8	0
20	Os cem anos do Ã¡tomo de Sommerfeld. Revista Brasileira De Ensino De Fisica, 2016, 38, .	0.2	0
21	A generalized Mittag-Leffler function to describe nonexponential chemical effects. Applied Mathematical Modelling, 2016, 40, 7971-7976.	4.2	11
22	Accurate multi-reference study of Si3 electronic manifold. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	2
23	TRANSMISSION AND REFLECTION COEFFICIENTS BY THE VARIABLE AMPLITUDE METHOD. Quimica Nova, 2016, , .	0.3	2
24	ILL-POSED INVERSE PROBLEMS IN CHEMISTRY. Quimica Nova, 2016, , .	0.3	1
25	Dataset structure as prior information for parameter-free regularization of extreme learning machines. Neurocomputing, 2015, 169, 288-294.	5.9	12
26	Variable phase equation in quantum scattering. Revista Brasileira De Ensino De Fisica, 2014, 36, .	0.2	6
27	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
28	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
29	Potential energy function information from quantum phase shift using the variable phase method. Journal of Molecular Modeling, 2014, 20, 2317.	1.8	2
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: 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
32	Methane combustion kinetic rate constants determination: an ill-posed inverse problem analysis. Quimica Nova, 2013, 36, 262-266.	0.3	2
33	O centenÃ¡rio da Teoria de Bohr. Quimica Nova, 2013, 36, 1073-1077.	0.3	0
34	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
35	Quantum Second Virial Coefficient Calculation for the⁴He Dimer on a Recent Potential. Journal of the Brazilian Chemical Society, 2013, , .	0.6	1
36	O centenÃ¡rio da molÃ©cula de Bohr. Quimica Nova, 2013, 36, 1078-1082.	0.3	1

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37	MÃ¡xima absorÃ§Ã£o ressonante em espectroscopia MÃ¶ssbauer. Revista Brasileira De Ensino De Fisica, 2013, 35, .	0.2	0
38	A kinetic study of jack-bean urease denaturation by a new dithiocarbamate bismuth compound. Chemical Physics Letters, 2012, 548, 85-89.	2.6	6
39	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
40	From deflection function to potential energy: A Firsov approach critical analysis. International Journal of Quantum Chemistry, 2012, 112, 3141-3146.	2.0	0
41	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
42	Parametric sensitivity analysis for the helium dimers on a model potential. Quimica Nova, 2012, 35, 910-913.	0.3	1
43	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
44	Hyperfine structure of 57Fe in minerals from a manganese ore deposit. Hyperfine Interactions, 2011, 203, 25-31.	0.5	0
45	Aspectos histÃ³ricos da visita de Marie Sklodowska Curie a Belo Horizonte. Quimica Nova, 2011, 34, 1888-1891.	0.3	0
46	O efeito de Coriolis: de pÃªndulos a molÃ©culas. Quimica Nova, 2010, 33, 1416-1420.	0.3	1
47	Ion-polymer interaction analysis: an inversion of NMR spin echo experimental data. Brazilian Journal of Physics, 2010, 40, .	1.4	2
48	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
49	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
50	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
51	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
52	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
53	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
54	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

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55	Coriolis coupling effects on energy transfer: classical-trajectories analysis for CO2 + Ar collisions. Canadian Journal of Chemistry, 2007, 85, 983-988.	1.1	3
56	A general algorithm to solve linear and nonlinear inverse problems. Journal of the Brazilian Chemical Society, 2007, 18, 1342-1347.	0.6	11
57	Coordenadas cartesianas moleculares a partir da geometria dos modos normais de vibraÃ§Ã£o. Quimica Nova, 2007, 30, 497-500.	0.3	3
58	Potential energy function from second virial data using sensitivity analysis. Inverse Problems in Science and Engineering, 2006, 14, 581-587.	1.2	6
59	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
60	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
61	Macromolecular properties from light-scattering experimental data using linear inverse problem theory. International Journal of Quantum Chemistry, 2006, 106, 2731-2736.	2.0	5
62	Force field inverse problems using recurrent neural networks. Chemical Physics Letters, 2006, 423, 357-360.	2.6	9
63	Diffusion coefficient distribution from NMR-DOSY experiments using Hopfield neural network. Journal of Magnetic Resonance, 2006, 182, 22-28.	2.1	27
64	Applications of genetic algorithms for inverting positron lifetime spectrum. Chemical Physics Letters, 2005, 412, 353-358.	2.6	2
65	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
66	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
67	Probability density function from experimental positron annihilation lifetime spectra. Journal of the Brazilian Chemical Society, 2005, 16, 93-97.	0.6	6
68	ReflexÃµes sobre a contribuiÃ§Ã£o da Carnot Ã primeira lei da termodinÃ¢mica. Quimica Nova, 2004, 27, 513-515.	0.3	3
69	Competition between kinetic models in thermal decomposition: analysis by artificial neural network. Thermochimica Acta, 2004, 412, 107-111.	2.7	29
70	Artificial neural network applied to solid state thermal decomposition. Journal of Thermal Analysis and Calorimetry, 2003, 74, 811-818.	3.6	20
71	Nonlinear global inversion of potential energy surfaces from the experimentally determined second virial coefficients. Chemical Physics Letters, 2003, 378, 406-409.	2.6	12
72	Inversion of simulated positron annihilation lifetime spectra by moving boundary subspaces. International Journal of Quantum Chemistry, 2003, 95, 97-102.	2.0	0

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73	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
74	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
75	Classical analysis of intermolecular potentials for ArÂ–CO2 rotational collisions. Canadian Journal of Chemistry, 2001, 79, 211-220.	1.1	0
76	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
77	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
78	Colapso da equipartiÃ§Ã£o da energia. Quimica Nova, 2001, 24, 693-699.	0.3	1
79	Title is missing!. Journal of Mathematical Chemistry, 2001, 29, 151-161.	1.5	15
80	TRAINING SVMs WITH EDR ALGORITHM. International Journal of Neural Systems, 2001, 11, 257-263.	5.2	1
81	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
82	Unified description of chemical bonding in H2 isotopomers, including Ps2, Î¼2 and bi-excitons. Chemical Physics Letters, 2000, 332, 139-144.	2.6	21
83	Hopfield neural network model for calculating the potential energy function from second virial data. Chemical Physics, 2000, 260, 347-352.	1.9	16
84	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
85	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
86	Classical trajectory study on Arâˆ’Cl2 van der Waals system using a recent potential. Chemical Physics, 1999, 241, 305-311.	1.9	1
87	Analysis of state-to-state classical rotational cross-sections for Arâ€“CO2 collisions. Physical Chemistry Chemical Physics, 1999, 1, 23-27.	2.8	3
88	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
89	A formulaÃ§Ã£o ab-initio da segunda lei da termodinÃ¢mica. Quimica Nova, 1998, 21, 499-503.	0.3	0
90	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

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91	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
92	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
93	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
94	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
95	A route to inversion for rotational collisions using hard shape potentials. Chemical Physics, 1996, 205, 401-406.	1.9	2
96	A critical analysis of the two-dimensional atom ellipsoid model to study rotational collisions. Chemical Physics, 1996, 213, 303-311.	1.9	4
97	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
98	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
99	The symmetrization in the classical path approach applied to vibrational cross sections. Chemical Physics, 1995, 200, 137-140.	1.9	0
100	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
101	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
102	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
103	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
104	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
105	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
106	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
107	The bound, metastable and virtual states of rare gas hydrides. Molecular Physics, 1984, 53, 295-299.	1.7	7
108	Complete Cl calculations on the ground state of HeH. Chemical Physics Letters, 1984, 110, 40-42.	2.6	16

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109	Artificial neural networks applied to theoretical chemistry. , 0, , .		0
110	SVM-KM: speeding SVMs learning with a priori cluster selection and k-means. , 0, , .		74
111	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
112	THE HYLLERAAS METHOD FOR TWO ELECTRONS ATOMS. Quimica Nova, 0, , .	0.3	1
113	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
114	Max Planckâ€™s Determination of the Avogadro Constant. Revista Brasileira De Ensino De Fisica, 0, 44, .	0.2	0