Geraldo M E Silva

List of Publications by Year
in descending order

59	688	567281	610901
papers	citations	15 h-index	24 g-index

59	59	59	430
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Dynamical evolution of polaron to bipolaron in conjugated polymers. Physical Review B, 2006, 74, .	3.2	53
2	Effects of temperature and electric field induced phase transitions on the dynamics of polarons and bipolarons. New Journal of Chemistry, 2013, 37, 2829.	2.8	48
3	Electronâ€“Lattice Coupling in Armchair Graphene Nanoribbons. Journal of Physical Chemistry Letters, 2012, 3, 3039-3042.	4.6	41
4	Theoretical investigation of carotenoid ultraviolet spectra. International Journal of Quantum Chemistry, 2009, 109, 739-745.	2.0	35
5	Exciton dissociation and charge carrier recombination processes in organic semiconductors. Journal of Chemical Physics, 2011, 135, 224901.	3.0	34
6	Use of polarons and bipolarons in logical switches based on conjugated polymers. Physical Review B, 2002, 65, .	3.2	33
7	Dynamics of solitons in polyacetylene with interchain coupling. Physical Review B, 1993, 47, 12568-12577.	3.2	29
8	CO₂ adsorption on single-walled boron nitride nanotubes containing vacancy defects. RSC Advances, 2015, 5, 27412-27420.	3.6	28
9	Theoretical Temperature Dependence of the Charge-Carrier Mobility in Semiconducting Polymers. Journal of Physical Chemistry A, 2009, 113, 14591-14594.	2.5	24
10	Thermal effects on photogeneration of free carriers in organic conductors. Chemical Physics Letters, 2010, 493, 283-287.	2.6	22
11	Polaron Properties in Armchair Graphene Nanoribbons. Journal of Physical Chemistry A, 2016, 120, 4893-4900.	2.5	21
12	Impurity effects and temperature influence on the exciton dissociation dynamics in conjugated polymers. Chemical Physics Letters, 2013, 580, 108-114.	2.6	20
13	Vibrational and Electronic Structure Analysis of a Carbon Dioxide Interaction with Functionalized Single-Walled Carbon Nanotubes. Journal of Physical Chemistry A, 2013, 117, 2854-2861.	2.5	20
14	Charge carrier untrapping by temperature effects in conjugated polymers. Europhysics Letters, 2009, 88, 67006.	2.0	18
15	Rovibrational energies and spectroscopic constants for H2Oâ‹¯Ng complexes. Journal of Molecular Modeling, 2014, 20, 2498.	1.8	17
16	Theoretical calculations of a new potential energy surface for the H + Li2 reaction. Chemical Physics Letters, 2010, 490, 123-126.	2.6	16
17	Molecular Dynamics Investigation of Charge Carrier Density Influence over Mobility in Conjugated Polymers. Journal of Physical Chemistry A, 2009, 113, 14975-14978.	2.5	15
18	Predicting the equilibrium structure of organic semiconductors with genetic algorithms. Chemical Physics Letters, 2013, 555, 168-172.	2.6	15

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19	Fitting potential energy surface of reactive systems via genetic algorithm. International Journal of Quantum Chemistry, 2006, 106, 2650-2657.	2.0	14
20	The H + Li2 bimolecular exchange reaction: Dynamical and kinetical properties at J = 0. Journal of Chemical Physics, 2012, 136, 134319.	3.0	14
21	Dynamics of Photogenerated Polaron-Excitons in Organic Semiconductors. Physics Procedia, 2012, 28, 112-116.	1.2	14
22	Spectroscopic properties of the molecular ion in the 8kÏ€, 9kÏƒ, 9lÏ€, 9lÏƒ and 10oÏƒ electronic states. Journal of Molecular Spectroscopy, 2012, 273, 26-29.	1.2	13
23	Temperature effects on polaron stability in polyacetylene. International Journal of Quantum Chemistry, 2008, 108, 2448-2453.	2.0	12
24	Dynamics of polarons and bipolarons with interchain coupling in conjugated polymers. International Journal of Quantum Chemistry, 2003, 95, 153-158.	2.0	10
25	A genetic algorithm to build diatomic potentials. Computational and Theoretical Chemistry, 2006, 769, 47-51.	1.5	9
26	Investigation of the Abstraction and Dissociation Mechanism in the Nitrogen Trifluoride Channels: Combined Post-Hartreeâ€“Fock and Transition State Theory Approaches. Journal of Physical Chemistry A, 2016, 120, 5464-5473.	2.5	9
27	Temperature-induced oscillating electric dipole in conjugated systems. Chemical Physics Letters, 2012, 539-540, 214-217.	2.6	8
28	Quantum Monte Carlo and genetic algorithm study of the potential energy surface of the H molecule. International Journal of Quantum Chemistry, 2008, 108, 2318-2325.	2.0	7
29	Dynamical properties and thermal rate coefficients for the Na + HF reaction using genetic algorithm. International Journal of Quantum Chemistry, 2010, 110, 1070-1079.	2.0	7
30	Supersonic quasi-particles dynamics in organic semiconductors. Chemical Physics Letters, 2012, 550, 146-149.	2.6	7
31	Polaron stability under collision with different defects in conjugated polymers. International Journal of Quantum Chemistry, 2006, 106, 2603-2608.	2.0	5
32	Thermal rate coefficients calculation for the H⁺ + LiH reaction. International Journal of Quantum Chemistry, 2010, 110, 2024-2028.	2.0	5
33	Dynamics of charge propagation on molecular circuits. Computational and Theoretical Chemistry, 1999, 464, 67-72.	1.5	4
34	Logical switching with the use of bipolarons in conjugated polymers. Computational and Theoretical Chemistry, 2001, 539, 55-64.	1.5	4
35	Dynamic interaction between polarons and torsional vibrations in conjugated polymers. International Journal of Quantum Chemistry, 2005, 103, 604-609.	2.0	4
36	Rovibrational energies and spectroscopic constants of the H system in the electronic states 1SÏƒ, 7iÏƒ, 5fÏ€, 5gÏ€, 6iÏ€, and 6iÏ•. International Journal of Quantum Chemistry, 2008, 108, 2398-2402.	2.0	4

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37	Thermal Rate Constant Calculation of the NF + F Reactive System Multiple Arrangements. Journal of Physical Chemistry A, 2011, 115, 8248-8254.	2.5	4
38	A detailed reactive cross section study of X + Li2 â†' Li + LiX, with X = H, D, T, and Mu. Journal of Molecular Modeling, 2014, 20, 2315.	1.8	4
39	Predicting New Pathways for the Reaction CN + C2H2. Revista Virtual De Quimica, 2016, 8, 515-524.	0.4	4
40	Dynamical effects on the competition between polarons and bipolarons in conjugated polymers. Computational and Theoretical Chemistry, 2001, 539, 45-53.	1.5	3
41	Linking model Hamiltonians to ab initio and semiempirical methods in descriptions of impurities in conjugated polymers. International Journal of Quantum Chemistry, 2005, 103, 537-542.	2.0	3
42	Effects of impurities on polaron dynamics in conjugated polymers: Effective potentials. International Journal of Quantum Chemistry, 2006, 106, 2597-2602.	2.0	3
43	Dynamics of photoexcitations with interchain coupling in conjugated polymers. International Journal of Quantum Chemistry, 2008, 108, 2442-2447.	2.0	3
44	Photo-generation of polaron pairs in coupled chains of polyacetylene. Computational and Theoretical Chemistry, 2008, 852, 11-14.	1.5	3
45	A Computational Investigation of the Multiple Channels of the NF2 + F Reaction. Journal of Physical Chemistry A, 2009, 113, 14336-14342.	2.5	3
46	H₂O₂â€“Ng dynamics predictions using an accurate potential energy surface. Molecular Physics, 0, , 1-6.	1.7	3
47	A moving soliton in the TLM model. Synthetic Metals, 1991, 43, 3713-3716.	3.9	2
48	Nonlinear excitations dynamics in molecular switches. Synthetic Metals, 1997, 86, 2245-2246.	3.9	2
49	Interaction of Torsional Oscillations with Polarons and Bipolarons in Conjugated Polymer. Synthetic Metals, 2005, 153, 493-496.	3.9	2
50	Chain length effects on nonlinear excitation transitions in transâ€polyacetylene. International Journal of Quantum Chemistry, 2008, 108, 2507-2511.	2.0	2
51	H₂⁺ dynamical properties in the electronic states 7jÏƒ, 8jÏƒ, 8kÏƒ, 7iÏ€, and 8jp. International Journal of Quantum Chemistry, 2011, 111, 1316-1320.	2.0	2
52	Competition between polarons and bipolarons â€" doping and electric field dynamical effects. Synthetic Metals, 2001, 119, 225-226.	3.9	1
53	Quantum bits with polyacetylene. Journal of Computational Chemistry, 2002, 23, 870-873.	3.3	1
54	Structural phases of coupled polyacetylene chains with impurities. International Journal of Quantum Chemistry, 2005, 103, 597-603.	2.0	1

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55	Quantum-controlled NOT gate made of coupled polyacetylene chains. International Journal of Quantum Chemistry, 2005, 103, 543-549.	2.0	1
56	Quantum reactive study of a potential energy surface obtained via genetic algorithm. International Journal of Quantum Chemistry, 2008, 108, 2306-2311.	2.0	1
57	Bosonic Charge Carriers in Necklace-like Graphene Nanoribbons. Journal of Physical Chemistry Letters, 2020, 11, 5538-5543.	4.6	1
58	Impurity effects on solitons in conjugated polymer linking model hamiltonians and ab initio method descriptions. Computational and Theoretical Chemistry, 2006, 769, 33-37.	1.5	0
59	Influence of the photoexcitation process on the dynamics of triplet excitons in organic polymers. Computational and Theoretical Chemistry, 2013, 1018, 91-94.	2.5	0