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	Bosonic Charge Carriers in Necklace-like Graphene Nanoribbons. Journal of Physical Chemistry Letters, 2020, 11, 5538-5543.	4.6	1
2	Polaron Properties in Armchair Graphene Nanoribbons. Journal of Physical Chemistry A, 2016, 120, 4893-4900.	2.5	21
3	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
4	Predicting New Pathways for the Reaction CN + C2H2. Revista Virtual De Quimica, 2016, 8, 515-524.	0.4	4
5	CO₂ adsorption on single-walled boron nitride nanotubes containing vacancy defects. RSC Advances, 2015, 5, 27412-27420.	3.6	28
6	Rovibrational energies and spectroscopic constants for H2Oâˆ’Ng complexes. Journal of Molecular Modeling, 2014, 20, 2498.	1.8	17
7	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
8	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
9	Impurity effects and temperature influence on the exciton dissociation dynamics in conjugated polymers. Chemical Physics Letters, 2013, 580, 108-114.	2.6	20
10	Predicting the equilibrium structure of organic semiconductors with genetic algorithms. Chemical Physics Letters, 2013, 555, 168-172.	2.6	15
11	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
12	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
13	Supersonic quasi-particles dynamics in organic semiconductors. Chemical Physics Letters, 2012, 550, 146-149.	2.6	7
14	Electronâ€“Lattice Coupling in Armchair Graphene Nanoribbons. Journal of Physical Chemistry Letters, 2012, 3, 3039-3042.	4.6	41
15	Temperature-induced oscillating electric dipole in conjugated systems. Chemical Physics Letters, 2012, 539-540, 214-217.	2.6	8
16	The H + Li2 bimolecular exchange reaction: Dynamical and kinetical properties at J = 0. Journal of Chemical Physics, 2012, 136, 134319.	3.0	14
17	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
18	Dynamics of Photogenerated Polaron-Excitons in Organic Semiconductors. Physics Procedia, 2012, 28, 112-116.	1.2	14

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19	Thermal Rate Constant Calculation of the NF + F Reactive System Multiple Arrangements. Journal of Physical Chemistry A, 2011, 115, 8248-8254.	2.5	4
20	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
21	Exciton dissociation and charge carrier recombination processes in organic semiconductors. Journal of Chemical Physics, 2011, 135, 224901.	3.0	34
22	Theoretical calculations of a new potential energy surface for the H + Li2 reaction. Chemical Physics Letters, 2010, 490, 123-126.	2.6	16
23	Thermal effects on photogeneration of free carriers in organic conductors. Chemical Physics Letters, 2010, 493, 283-287.	2.6	22
24	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
25	Thermal rate coefficients calculation for the H⁺ + LiH reaction. International Journal of Quantum Chemistry, 2010, 110, 2024-2028.	2.0	5
26	Theoretical Temperature Dependence of the Charge-Carrier Mobility in Semiconducting Polymers. Journal of Physical Chemistry A, 2009, 113, 14591-14594.	2.5	24
27	A Computational Investigation of the Multiple Channels of the NF2 + F Reaction. Journal of Physical Chemistry A, 2009, 113, 14336-14342.	2.5	3
28	Charge carrier untrapping by temperature effects in conjugated polymers. Europhysics Letters, 2009, 88, 67006.	2.0	18
29	Theoretical investigation of carotenoid ultraviolet spectra. International Journal of Quantum Chemistry, 2009, 109, 739-745.	2.0	35
30	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
31	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
32	Quantum reactive study of a potential energy surface obtained via genetic algorithm. International Journal of Quantum Chemistry, 2008, 108, 2306-2311.	2.0	1
33	Chain length effects on nonlinear excitation transitions in transâ€polyacetylene. International Journal of Quantum Chemistry, 2008, 108, 2507-2511.	2.0	2
34	Dynamics of photoexcitations with interchain coupling in conjugated polymers. International Journal of Quantum Chemistry, 2008, 108, 2442-2447.	2.0	3
35	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
36	Temperature effects on polaron stability in polyacetylene. International Journal of Quantum Chemistry, 2008, 108, 2448-2453.	2.0	12

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37	Photo-generation of polaron pairs in coupled chains of polyacetylene. Computational and Theoretical Chemistry, 2008, 852, 11-14.	1.5	3
38	Effects of impurities on polaron dynamics in conjugated polymers: Effective potentials. International Journal of Quantum Chemistry, 2006, 106, 2597-2602.	2.0	3
39	Polaron stability under collision with different defects in conjugated polymers. International Journal of Quantum Chemistry, 2006, 106, 2603-2608.	2.0	5
40	Fitting potential energy surface of reactive systems via genetic algorithm. International Journal of Quantum Chemistry, 2006, 106, 2650-2657.	2.0	14
41	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
42	A genetic algorithm to build diatomic potentials. Computational and Theoretical Chemistry, 2006, 769, 47-51.	1.5	9
43	Dynamical evolution of polaron to bipolaron in conjugated polymers. Physical Review B, 2006, 74, .	3.2	53
44	Structural phases of coupled polyacetylene chains with impurities. International Journal of Quantum Chemistry, 2005, 103, 597-603.	2.0	1
45	Quantum-controlled NOT gate made of coupled polyacetylene chains. International Journal of Quantum Chemistry, 2005, 103, 543-549.	2.0	1
46	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
47	Dynamic interaction between polarons and torsional vibrations in conjugated polymers. International Journal of Quantum Chemistry, 2005, 103, 604-609.	2.0	4
48	Interaction of Torsional Oscillations with Polarons and Bipolarons in Conjugated Polymer. Synthetic Metals, 2005, 153, 493-496.	3.9	2
49	Dynamics of polarons and bipolarons with interchain coupling in conjugated polymers. International Journal of Quantum Chemistry, 2003, 95, 153-158.	2.0	10
50	Use of polarons and bipolarons in logical switches based on conjugated polymers. Physical Review B, 2002, 65, .	3.2	33
51	Quantum bits with polyacetylene. Journal of Computational Chemistry, 2002, 23, 870-873.	3.3	1
52	Competition between polarons and bipolarons â€" doping and electric field dynamical effects. Synthetic Metals, 2001, 119, 225-226.	3.9	1
53	Dynamical effects on the competition between polarons and bipolarons in conjugated polymers. Computational and Theoretical Chemistry, 2001, 539, 45-53.	1.5	3
54	Logical switching with the use of bipolarons in conjugated polymers. Computational and Theoretical Chemistry, 2001, 539, 55-64.	1.5	4

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55	Dynamics of charge propagation on molecular circuits. Computational and Theoretical Chemistry, 1999, 464, 67-72.	1.5	4
56	Nonlinear excitations dynamics in molecular switches. Synthetic Metals, 1997, 86, 2245-2246.	3.9	2
57	Dynamics of solitons in polyacetylene with interchain coupling. Physical Review B, 1993, 47, 12568-12577.	3.2	29
58	A moving soliton in the TLM model. Synthetic Metals, 1991, 43, 3713-3716.	3.9	2
59	H₂O₂â€“Ng dynamics predictions using an accurate potential energy surface. Molecular Physics, 0, , 1-6.	1.7	3