Geraldo M E Silva

List of Publications by Year in Descending Order

57 papers	609 citations	15 h-index	22 g-index
59 ext. papers	632 ext. citations	2.6 avg, IF	3.58 L-index

#	Paper	IF	Citations
57	Bosonic Charge Carriers in Necklace-like Graphene Nanoribbons. *Journal of Physical Chemistry Letters*, **2020**, 11, 5538-5543	6.4	1
56	Polaron Properties in Armchair Graphene Nanoribbons. *Journal of Physical Chemistry A*, **2016**, 120, 4893-900	2.8	18
55	Investigation of the Abstraction and Dissociation Mechanism in the Nitrogen Trifluoride Channels: Combined Post-Hartree-Fock and Transition State Theory Approaches. *Journal of Physical Chemistry A*, **2016**, 120, 5464-73	2.8	8
54	CO2 adsorption on single-walled boron nitride nanotubes containing vacancy defects. *RSC Advances*, **2015**, 5, 27412-27420	3.7	23
53	H2O2Ng dynamics predictions using an accurate potential energy surface. *Molecular Physics*, **2015**, 1-6	1.7	1
52	A detailed reactive cross section study of X + Li2 -Li + LiX, with X = H, D, T, and Mu. *Journal of Molecular Modeling*, **2014**, 20, 2315	2	3
51	Rovibrational energies and spectroscopic constants for H2O-Ng complexes. *Journal of Molecular Modeling*, **2014**, 20, 2498	2	13
50	Effects of temperature and electric field induced phase transitions on the dynamics of polarons and bipolarons. *New Journal of Chemistry*, **2013**, 37, 2829	3.6	41
49	Impurity effects and temperature influence on the exciton dissociation dynamics in conjugated polymers. *Chemical Physics Letters*, **2013**, 580, 108-114	2.5	19
48	Predicting the equilibrium structure of organic semiconductors with genetic algorithms. *Chemical Physics Letters*, **2013**, 555, 168-172	2.5	15
47	Influence of the photoexcitation process on the dynamics of triplet excitons in organic polymers. *Computational and Theoretical Chemistry*, **2013**, 1018, 91-94	2	
46	Vibrational and electronic structure analysis of a carbon dioxide interaction with functionalized single-walled carbon nanotubes. *Journal of Physical Chemistry A*, **2013**, 117, 2854-61	2.8	17
45	Spectroscopic properties of the molecular ion in the 8k9k9l9l and 10o electronic states. *Journal of Molecular Spectroscopy*, **2012**, 273, 26-29	1.3	11
44	Dynamics of Photogenerated Polaron-Excitons in Organic Semiconductors. *Physics Procedia*, **2012**, 28, 112-116		14
43	Supersonic quasi-particles dynamics in organic semiconductors. *Chemical Physics Letters*, **2012**, 550, 146-149	2.5	5
42	Electron-Lattice Coupling in Armchair Graphene Nanoribbons. *Journal of Physical Chemistry Letters*, **2012**, 3, 3039-42	6.4	36
41	Temperature-induced oscillating electric dipole in conjugated systems. *Chemical Physics Letters*, **2012**, 539-540, 214-217	2.5	8

40	The H + Li2 bimolecular exchange reaction: dynamical and kinetical properties at J = 0. *Journal of Chemical Physics*, **2012**, 136, 134319	3.9	14
39	H2+ dynamical properties in the electronic states 7j□8j□8k□7i□and 8jp. *International Journal of Quantum Chemistry*, **2011**, 111, 1316-1320	2.1	2
38	Thermal rate constant calculation of the NF + F reactive system multiple arrangements. *Journal of Physical Chemistry A*, **2011**, 115, 8248-54	2.8	2
37	Exciton dissociation and charge carrier recombination processes in organic semiconductors. *Journal of Chemical Physics*, **2011**, 135, 224901	3.9	30
36	Theoretical calculations of a new potential energy surface for the H + Li2 reaction. *Chemical Physics Letters*, **2010**, 490, 123-126	2.5	15
35	Thermal effects on photogeneration of free carriers in organic conductors. *Chemical Physics Letters*, **2010**, 493, 283-287	2.5	22
34	Dynamical properties and thermal rate coefficients for the Na + HF reaction using genetic algorithm. *International Journal of Quantum Chemistry*, **2010**, 110, 1070-1079	2.1	3
33	Thermal rate coefficients calculation for the H+ + LiH reaction. *International Journal of Quantum Chemistry*, **2010**, 110, 2024-2028	2.1	5
32	Theoretical temperature dependence of the charge-carrier mobility in semiconducting polymers. *Journal of Physical Chemistry A*, **2009**, 113, 14591-4	2.8	20
31	A computational investigation of the multiple channels of the NF2 + F reaction. *Journal of Physical Chemistry A*, **2009**, 113, 14336-42	2.8	3
30	Charge carrier untrapping by temperature effects in conjugated polymers. *Europhysics Letters*, **2009** , 88, 67006	1.6	16
29	Theoretical investigation of carotenoid ultraviolet spectra. *International Journal of Quantum Chemistry*, **2009**, 109, 739-745	2.1	34
28	Molecular dynamics investigation of charge carrier density influence over mobility in conjugated polymers. *Journal of Physical Chemistry A*, **2009**, 113, 14975-8	2.8	15
27	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	2.1	6
26	Quantum reactive study of a potential energy surface obtained via genetic algorithm. *International Journal of Quantum Chemistry*, **2008**, 108, 2306-2311	2.1	0
25	Chain length effects on nonlinear excitation transitions in trans-polyacetylene. *International Journal of Quantum Chemistry*, **2008**, 108, 2507-2511	2.1	2
24	Dynamics of photoexcitations with interchain coupling in conjugated polymers. *International Journal of Quantum Chemistry*, **2008**, 108, 2442-2447	2.1	3
23	Rovibrational energies and spectroscopic constants of the H system in the electronic states 1S□ 7i□5f□5g□6i□and 6i?. *International Journal of Quantum Chemistry*, **2008**, 108, 2398-2402	2.1	4

22	Temperature effects on polaron stability in polyacetylene. *International Journal of Quantum Chemistry*, **2008**, 108, 2448-2453	2.1	10
21	Photo-generation of polaron pairs in coupled chains of polyacetylene. *Computational and Theoretical Chemistry*, **2008**, 852, 11-14		3
20	Dynamical evolution of polaron to bipolaron in conjugated polymers. *Physical Review B*, **2006**, 74,	3.3	50
19	Effects of impurities on polaron dynamics in conjugated polymers: Effective potentials. *International Journal of Quantum Chemistry*, **2006**, 106, 2597-2602	2.1	3
18	Polaron stability under collision with different defects in conjugated polymers. *International Journal of Quantum Chemistry*, **2006**, 106, 2603-2608	2.1	3
17	Fitting potential energy surface of reactive systems via genetic algorithm. *International Journal of Quantum Chemistry*, **2006**, 106, 2650-2657	2.1	10
16	Impurity effects on solitons in conjugated polymer linking model hamiltonians and ab initio method descriptions. *Computational and Theoretical Chemistry*, **2006**, 769, 33-37		
15	A genetic algorithm to build diatomic potentials. *Computational and Theoretical Chemistry*, **2006**, 769, 47-51		8
14	Interaction of Torsional Oscillations with Polarons and Bipolarons in Conjugated Polymer. *Synthetic Metals*, **2005**, 153, 493-496	3.6	2
13	Structural phases of coupled polyacetylene chains with impurities. *International Journal of Quantum Chemistry*, **2005**, 103, 597-603	2.1	1
12	Quantum-controlled NOT gate made of coupled polyacetylene chains. *International Journal of Quantum Chemistry*, **2005**, 103, 543-549	2.1	1
11	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	2.1	3
10	Dynamic interaction between polarons and torsional vibrations in conjugated polymers. *International Journal of Quantum Chemistry*, **2005**, 103, 604-609	2.1	4
9	Dynamics of polarons and bipolarons with interchain coupling in conjugated polymers. *International Journal of Quantum Chemistry*, **2003**, 95, 153-158	2.1	9
8	Quantum bits with polyacetylene. *Journal of Computational Chemistry*, **2002**, 23, 870-3	3.5	1
7	Use of polarons and bipolarons in logical switches based on conjugated polymers. *Physical Review B* , **2002**, 65,	3.3	32
6	Dynamical effects on the competition between polarons and bipolarons in conjugated polymers. *Computational and Theoretical Chemistry*, **2001**, 539, 45-53		
5	Logical switching with the use of bipolarons in conjugated polymers. *Computational and Theoretical Chemistry*, **2001**, 539, 55-64		4

4	Dynamics of charge propagation on molecular circuits. *Computational and Theoretical Chemistry*, **1999**, 464, 67-72		4
3	Nonlinear excitations dynamics in molecular switches. *Synthetic Metals*, **1997**, 86, 2245-2246	3.6	2
2	Dynamics of solitons in polyacetylene with interchain coupling. *Physical Review B*, **1993**, 47, 12568-12577	3.3	26
1	A moving soliton in the TLM model. *Synthetic Metals*, **1991**, 43, 3713-3716	3.6	2