Geraldo Magela E Silva

List of Publications by Year
in descending order

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93 papers	1,013 citations	516710 16 h-index	552781 26 g-index
93 all docs	93 docs citations	93 times ranked	458 citing authors

#	Article	IF	Citations
1	Charge transport in cove-type graphene nanoribbons: The role of quasiparticles. Synthetic Metals, 2022, 287, 117056.	3.9	8
2	Quasiparticle dynamics by effective $$pi $$-field distortion. Scientific Reports, 2022, 12, 7967.	3.3	4
3	Charge localization and hopping in a topologically engineered graphene nanoribbon. Scientific Reports, 2021, 11, 5142.	3.3	5
4	Ultrafast direct generation of quasiparticles in graphene nanoribbons. Carbon, 2020, 158, 553-558.	10.3	15
5	Charge Transport Mechanism in Chevron-Graphene Nanoribbons. Journal of Physical Chemistry C, 2020, 124, 22392-22398.	3.1	3
6	Smooth gap tuning strategy for cove-type graphene nanoribbons. RSC Advances, 2020, 10, 26937-26943.	3.6	10
7	Transport of quasiparticles in coronene-based graphene nanoribbons. Journal of Materials Chemistry C, 2020, 8, 12100-12107.	5.5	8
8	Stability conditions of armchair graphene nanoribbon bipolarons. Journal of Molecular Modeling, 2019, 25, 245.	1.8	8
9	Polaron properties in 2D organic molecular crystals: directional dependence of non-local electronâ€“phonon coupling. Journal of Molecular Modeling, 2019, 25, 149.	1.8	2
10	Electron-phonon coupling in armchair silicene nanoribbons. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 125954.	2.1	6
11	Same Charge Polaron and Bipolaron Scattering on Conducting Polymers. Journal of Physical Chemistry A, 2019, 123, 1319-1327.	2.5	8
12	Stationary polaron properties in organic crystalline semiconductors. Physical Chemistry Chemical Physics, 2019, 21, 2727-2733.	2.8	9
13	Tuning the electronic structure properties of MoS₂ monolayers with carbon doping. Physical Chemistry Chemical Physics, 2019, 21, 11168-11174.	2.8	10
14	Stationary and Dynamical Properties of Polarons in Anisotropic C₆₀-Crystals. Journal of Physical Chemistry C, 2019, 123, 13410-13418.	3.1	7
15	Fast predictions of exciton diffusion length in organic materials. Journal of Materials Chemistry C, 2019, 7, 4066-4071.	5.5	13
16	Bipolaron Dynamics in Graphene Nanoribbons. Scientific Reports, 2019, 9, 2909.	3.3	14
17	Modeling Polaron Diffusion in Oligoacene-like Crystals. Journal of Physical Chemistry C, 2019, 123, 4715-4720.	3.1	9
18	Dynamical Mechanism of Polarons and Bipolarons in Poly(p-Phenylene Vinylene). Scientific Reports, 2019, 9, 18131.	3.3	3

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19	Effective Mass of Quasiparticles in Armchair Graphene Nanoribbons. Scientific Reports, 2019, 9, 17990.	3.3	5
20	Concentration effects on the thermally-activated transport of polarons in conducting polymers. Chemical Physics Letters, 2019, 716, 162-166.	2.6	6
21	Quasiparticle description of transition metal dichalcogenide nanoribbons. Physical Review B, 2019, 99, .	3.2	8
22	Spin-Orbit Effects on the Dynamical Properties of Polarons in Graphene Nanoribbons. Scientific Reports, 2018, 8, 1914.	3.3	8
23	Charge Carrier Scattering in Polymers: A New Neutral Coupled Soliton Channel. Scientific Reports, 2018, 8, 6595.	3.3	5
24	Dynamic Formation of Bipolaronâ€“Exciton Complexes in Conducting Polymers. Journal of Physical Chemistry A, 2018, 122, 3866-3872.	2.5	1
25	Influence of quasi-particle density over polaron mobility in armchair graphene nanoribbons. Physical Chemistry Chemical Physics, 2018, 20, 16712-16718.	2.8	15
26	Electronâ€“phonon coupling effects on intrachain polaron recombination in conjugated polymers. Journal of Molecular Modeling, 2017, 23, 42.	1.8	2
27	Polaron and bipolaron stability on paraphenylene polymers. Journal of Molecular Modeling, 2017, 23, 59.	1.8	4
28	Bipolaron assisted Bloch-like oscillations in organic lattices. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 1915-1919.	2.1	4
29	Bloch oscillations in organic and inorganic polymers. Journal of Chemical Physics, 2017, 146, 144903.	3.0	3
30	Bond length pattern associated with charge carriers in armchair graphene nanoribbons. Journal of Molecular Modeling, 2017, 23, 293.	1.8	9
31	Low-Temperature Seebeck Coefficients for Polaron-Driven Thermoelectric Effect in Organic Polymers. Journal of Physical Chemistry A, 2016, 120, 4923-4927.	2.5	7
32	Impact of the Electronâ€“Phonon Interactions on the Polaron Dynamics in Graphene Nanoribbons. Journal of Physical Chemistry A, 2016, 120, 4901-4906.	2.5	19
33	Dynamics of charge carriers on hexagonal nanoribbons with vacancy defects. Physical Review B, 2016, 94, .	3.2	21
34	Transport of Polarons in Graphene Nanoribbons. Journal of Physical Chemistry Letters, 2015, 6, 510-514.	4.6	41
35	Concentration effects on intrachain polaron recombination in conjugated polymers. Physical Chemistry Chemical Physics, 2015, 17, 1299-1308.	2.8	7
36	Impurity effects on polaron dynamics in graphene nanoribbons. Carbon, 2015, 91, 171-177.	10.3	26

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37	Limit of Exciton Diffusion in Highly Ordered Ï€-Conjugated Systems. Journal of Physical Chemistry C, 2015, 119, 19654-19659.	3.1	10
38	Critical temperature and products of intrachain polaron recombination in conjugated polymers. Physical Chemistry Chemical Physics, 2014, 16, 17072-17080.	2.8	34
39	Temperature Effects on the Scattering of Polarons and Bipolarons in Organic Conductors. Journal of Physical Chemistry A, 2014, 118, 6272-6277.	2.5	11
40	Reactive Scattering between Excitons and Charge Carriers in Conjugated Polymers. Journal of Physical Chemistry C, 2014, 118, 23451-23458.	3.1	13
41	Singletâ€“Singlet Exciton Recombination: Theoretical Insight into the Influence of High Density Regime of Excitons in Conjugated Polymers. Journal of Physical Chemistry B, 2014, 118, 5250-5257.	2.6	8
42	Temperature effects on intrachain recombination of bipolarons in conjugated polymers. Chemical Physics Letters, 2014, 614, 151-155.	2.6	12
43	Carbon dioxide adsorption on doped boron nitride nanotubes. RSC Advances, 2014, 4, 28249-28258.	3.6	34
44	Influence of bipolaron density on the transport properties of thermalized organic conductors. International Journal of Quantum Chemistry, 2013, 113, 2540-2545.	2.0	2
45	An extensive investigation of reactions involved in the nitrogen trifluoride dissociation. New Journal of Chemistry, 2013, 37, 3244.	2.8	1
46	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
47	Predicting the equilibrium structure of organic semiconductors with genetic algorithms. Chemical Physics Letters, 2013, 555, 168-172.	2.6	15
48	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
49	Dynamical Study of Impurity Effects on Bipolaronâ€“Bipolaron and Bipolaronâ€“Polaron Scattering in Conjugated Polymers. Journal of Physical Chemistry B, 2013, 117, 11801-11811.	2.6	20
50	Impurity effects on polaron-exciton formation in conjugated polymers. Journal of Chemical Physics, 2013, 139, 174903.	3.0	18
51	Supersonic quasi-particles dynamics in organic semiconductors. Chemical Physics Letters, 2012, 550, 146-149.	2.6	7
52	The H + Li2 bimolecular exchange reaction: Dynamical and kinetical properties at J = 0. Journal of Chemical Physics, 2012, 136, 134319.	3.0	14
53	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
54	Thermal Rate Constant Calculation of the NF + F Reactive System Multiple Arrangements. Journal of Physical Chemistry A, 2011, 115, 8248-8254.	2.5	4

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55	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
56	Theoretical calculations of a new potential energy surface for the H + Li2 reaction. Chemical Physics Letters, 2010, 490, 123-126.	2.6	16
57	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
58	Theoretical Temperature Dependence of the Charge-Carrier Mobility in Semiconducting Polymers. Journal of Physical Chemistry A, 2009, 113, 14591-14594.	2.5	24
59	A Computational Investigation of the Multiple Channels of the NF2 + F Reaction. Journal of Physical Chemistry A, 2009, 113, 14336-14342.	2.5	3
60	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
61	Interchain interaction effects on polaronâ€“bipolaron transition on conducting polymers. Journal of Materials Science, 2008, 43, 585-590.	3.7	5
62	Chain length effects on nonlinear excitation transitions in transâ€polyacetylene. International Journal of Quantum Chemistry, 2008, 108, 2507-2511.	2.0	2
63	Dynamics of photoexcitations with interchain coupling in conjugated polymers. International Journal of Quantum Chemistry, 2008, 108, 2442-2447.	2.0	3
64	Temperature effects on polaron stability in polyacetylene. International Journal of Quantum Chemistry, 2008, 108, 2448-2453.	2.0	12
65	Photo-generation of polaron pairs in coupled chains of polyacetylene. Computational and Theoretical Chemistry, 2008, 852, 11-14.	1.5	3
66	Transition of polaron to bipolaron structure in conjugated polymers. Computational and Theoretical Chemistry, 2008, 852, 15-21.	1.5	4
67	Dynamics Simulation of Conducting Polymer Interchain Interaction Effects on Polaron Transition. Lecture Notes in Computer Science, 2007, , 304-311.	1.3	0
68	Effects of impurities on polaron dynamics in conjugated polymers: Effective potentials. International Journal of Quantum Chemistry, 2006, 106, 2597-2602.	2.0	3
69	Polaron stability under collision with different defects in conjugated polymers. International Journal of Quantum Chemistry, 2006, 106, 2603-2608.	2.0	5
70	Fitting potential energy surface of reactive systems via genetic algorithm. International Journal of Quantum Chemistry, 2006, 106, 2650-2657.	2.0	14
71	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
72	A genetic algorithm to build diatomic potentials. Computational and Theoretical Chemistry, 2006, 769, 47-51.	1.5	9

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73	Dynamical evolution of polaron to bipolaron in conjugated polymers. Physical Review B, 2006, 74, .	3.2	53
74	Structural phases of coupled polyacetylene chains with impurities. International Journal of Quantum Chemistry, 2005, 103, 597-603.	2.0	1
75	Quantum-controlled NOT gate made of coupled polyacetylene chains. International Journal of Quantum Chemistry, 2005, 103, 543-549.	2.0	1
76	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
77	Dynamic interaction between polarons and torsional vibrations in conjugated polymers. International Journal of Quantum Chemistry, 2005, 103, 604-609.	2.0	4
78	Interaction of Torsional Oscillations with Polarons and Bipolarons in Conjugated Polymer. Synthetic Metals, 2005, 153, 493-496.	3.9	2
79	Dynamics of polarons and bipolarons with interchain coupling in conjugated polymers. International Journal of Quantum Chemistry, 2003, 95, 153-158.	2.0	10
80	Polyacetylene as a qubit system. International Journal of Quantum Chemistry, 2003, 95, 224-229.	2.0	1
81	Use of polarons and bipolarons in logical switches based on conjugated polymers. Physical Review B, 2002, 65, .	3.2	33
82	Quantum bits with polyacetylene. Journal of Computational Chemistry, 2002, 23, 870-873.	3.3	1
83	Electric-field effects on the competition between polarons and bipolarons in conjugated polymers. Physical Review B, 2000, 61, 10777-10781.	3.2	83
84	Investigating charge transport in molecular switches with neural networks. Journal of Computational Chemistry, 1999, 20, 1060-1066.	3.3	5
85	Dynamics of charge transfer in molecular switches II. Effective potentials and Coulomb interaction. Synthetic Metals, 1998, 97, 195-203.	3.9	13
86	Dynamics of charge transfer in molecular switches. Synthetic Metals, 1997, 87, 249-256.	3.9	20
87	Nonlinear excitations dynamics in molecular switches. Synthetic Metals, 1997, 86, 2245-2246.	3.9	2
88	Collisions of solitons in polyacetylene. Computational and Theoretical Chemistry, 1997, 394, 161-167.	1.5	4
89	Estimating correlation energy of diatomic molecules and atoms with neural networks. Journal of Computational Chemistry, 1997, 18, 1407-1414.	3.3	17
90	Dynamics of conformational defects in poly(3-hexyl)thiophene. Physical Review B, 1996, 53, 7222-7226.	3.2	5

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91	Dynamics of solitons in polyacetylene with interchain coupling. Physical Review B, 1993, 47, 12568-12577.	3.2	29
92	Structure of the Moving Solitonin the TLM Model. Journal of the Physical Society of Japan, 1993, 62, 2745-2756.	1.6	0
93	A moving soliton in the TLM model. Synthetic Metals, 1991, 43, 3713-3716.	3.9	2