

Geraldo Magela E Silva

List of Publications by Year in descending order

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93
papers

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citations

516710

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93
docs citations

93
times ranked

458
citing authors

#	ARTICLE	IF	CITATIONS
1	Electric-field effects on the competition between polarons and bipolarons in conjugated polymers. <i>Physical Review B</i> , 2000, 61, 10777-10781.	3.2	83
2	Dynamical evolution of polaron to bipolaron in conjugated polymers. <i>Physical Review B</i> , 2006, 74, .	3.2	53
3	Effects of temperature and electric field induced phase transitions on the dynamics of polarons and bipolarons. <i>New Journal of Chemistry</i> , 2013, 37, 2829.	2.8	48
4	Transport of Polarons in Graphene Nanoribbons. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 510-514.	4.6	41
5	Critical temperature and products of intrachain polaron recombination in conjugated polymers. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17072-17080.	2.8	34
6	Carbon dioxide adsorption on doped boron nitride nanotubes. <i>RSC Advances</i> , 2014, 4, 28249-28258.	3.6	34
7	Use of polarons and bipolarons in logical switches based on conjugated polymers. <i>Physical Review B</i> , 2002, 65, .	3.2	33
8	Dynamics of solitons in polyacetylene with interchain coupling. <i>Physical Review B</i> , 1993, 47, 12568-12577.	3.2	29
9	Impurity effects on polaron dynamics in graphene nanoribbons. <i>Carbon</i> , 2015, 91, 171-177.	10.3	26
10	Theoretical Temperature Dependence of the Charge-Carrier Mobility in Semiconducting Polymers. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14591-14594.	2.5	24
11	Dynamics of charge carriers on hexagonal nanoribbons with vacancy defects. <i>Physical Review B</i> , 2016, 94, .	3.2	21
12	Dynamics of charge transfer in molecular switches. <i>Synthetic Metals</i> , 1997, 87, 249-256.	3.9	20
13	Dynamical Study of Impurity Effects on Bipolaronâ€“Bipolaron and Bipolaronâ€“Polaron Scattering in Conjugated Polymers. <i>Journal of Physical Chemistry B</i> , 2013, 117, 11801-11811.	2.6	20
14	Impact of the Electronâ€“Phonon Interactions on the Polaron Dynamics in Graphene Nanoribbons. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4901-4906.	2.5	19
15	Impurity effects on polaron-exciton formation in conjugated polymers. <i>Journal of Chemical Physics</i> , 2013, 139, 174903.	3.0	18
16	Estimating correlation energy of diatomic molecules and atoms with neural networks. <i>Journal of Computational Chemistry</i> , 1997, 18, 1407-1414.	3.3	17
17	Theoretical calculations of a new potential energy surface for the H + Li2 reaction. <i>Chemical Physics Letters</i> , 2010, 490, 123-126.	2.6	16
18	Molecular Dynamics Investigation of Charge Carrier Density Influence over Mobility in Conjugated Polymers. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14975-14978.	2.5	15

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19	Predicting the equilibrium structure of organic semiconductors with genetic algorithms. <i>Chemical Physics Letters</i> , 2013, 555, 168-172.	2.6	15
20	Influence of quasi-particle density over polaron mobility in armchair graphene nanoribbons. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 16712-16718.	2.8	15
21	Ultrafast direct generation of quasiparticles in graphene nanoribbons. <i>Carbon</i> , 2020, 158, 553-558.	10.3	15
22	Fitting potential energy surface of reactive systems via genetic algorithm. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2650-2657.	2.0	14
23	The H + Li ₂ bimolecular exchange reaction: Dynamical and kinetical properties at J = 0. <i>Journal of Chemical Physics</i> , 2012, 136, 134319.	3.0	14
24	Bipolaron Dynamics in Graphene Nanoribbons. <i>Scientific Reports</i> , 2019, 9, 2909.	3.3	14
25	Dynamics of charge transfer in molecular switches II. Effective potentials and Coulomb interaction. <i>Synthetic Metals</i> , 1998, 97, 195-203.	3.9	13
26	Spectroscopic properties of the molecular ion in the 8k ₁ g, 9k ₁ f, 9l ₁ g, 9l ₁ f and 10o ₁ f electronic states. <i>Journal of Molecular Spectroscopy</i> , 2012, 273, 26-29.	1.2	13
27	Reactive Scattering between Excitons and Charge Carriers in Conjugated Polymers. <i>Journal of Physical Chemistry C</i> , 2014, 118, 23451-23458.	3.1	13
28	Fast predictions of exciton diffusion length in organic materials. <i>Journal of Materials Chemistry C</i> , 2019, 7, 4066-4071.	5.5	13
29	Temperature effects on polaron stability in polyacetylene. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2448-2453.	2.0	12
30	Temperature effects on intrachain recombination of bipolarons in conjugated polymers. <i>Chemical Physics Letters</i> , 2014, 614, 151-155.	2.6	12
31	Temperature Effects on the Scattering of Polarons and Bipolarons in Organic Conductors. <i>Journal of Physical Chemistry A</i> , 2014, 118, 6272-6277.	2.5	11
32	Dynamics of polarons and bipolarons with interchain coupling in conjugated polymers. <i>International Journal of Quantum Chemistry</i> , 2003, 95, 153-158.	2.0	10
33	Limit of Exciton Diffusion in Highly Ordered π -Conjugated Systems. <i>Journal of Physical Chemistry C</i> , 2015, 119, 19654-19659.	3.1	10
34	Tuning the electronic structure properties of MoS ₂ monolayers with carbon doping. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 11168-11174.	2.8	10
35	Smooth gap tuning strategy for cove-type graphene nanoribbons. <i>RSC Advances</i> , 2020, 10, 26937-26943.	3.6	10
36	A genetic algorithm to build diatomic potentials. <i>Computational and Theoretical Chemistry</i> , 2006, 769, 47-51.	1.5	9

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37	Bond length pattern associated with charge carriers in armchair graphene nanoribbons. <i>Journal of Molecular Modeling</i> , 2017, 23, 293.	1.8	9
38	Stationary polaron properties in organic crystalline semiconductors. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2727-2733.	2.8	9
39	Modeling Polaron Diffusion in Oligoacene-like Crystals. <i>Journal of Physical Chemistry C</i> , 2019, 123, 4715-4720.	3.1	9
40	Singlet-Singlet Exciton Recombination: Theoretical Insight into the Influence of High Density Regime of Excitons in Conjugated Polymers. <i>Journal of Physical Chemistry B</i> , 2014, 118, 5250-5257.	2.6	8
41	Spin-Orbit Effects on the Dynamical Properties of Polarons in Graphene Nanoribbons. <i>Scientific Reports</i> , 2018, 8, 1914.	3.3	8
42	Stability conditions of armchair graphene nanoribbon bipolarons. <i>Journal of Molecular Modeling</i> , 2019, 25, 245.	1.8	8
43	Same Charge Polaron and Bipolaron Scattering on Conducting Polymers. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1319-1327.	2.5	8
44	Quasiparticle description of transition metal dichalcogenide nanoribbons. <i>Physical Review B</i> , 2019, 99, .	3.2	8
45	Transport of quasiparticles in coronene-based graphene nanoribbons. <i>Journal of Materials Chemistry C</i> , 2020, 8, 12100-12107.	5.5	8
46	Charge transport in cove-type graphene nanoribbons: The role of quasiparticles. <i>Synthetic Metals</i> , 2022, 287, 117056.	3.9	8
47	Dynamical properties and thermal rate coefficients for the $\text{Na} + \text{HF}$ reaction using genetic algorithm. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 1070-1079.	2.0	7
48	Supersonic quasi-particles dynamics in organic semiconductors. <i>Chemical Physics Letters</i> , 2012, 550, 146-149.	2.6	7
49	Concentration effects on intrachain polaron recombination in conjugated polymers. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 1299-1308.	2.8	7
50	Low-Temperature Seebeck Coefficients for Polaron-Driven Thermoelectric Effect in Organic Polymers. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4923-4927.	2.5	7
51	Stationary and Dynamical Properties of Polarons in Anisotropic C_{60} -Crystals. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13410-13418.	3.1	7
52	Electron-phonon coupling in armchair silicene nanoribbons. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019, 383, 125954.	2.1	6
53	Concentration effects on the thermally-activated transport of polarons in conducting polymers. <i>Chemical Physics Letters</i> , 2019, 716, 162-166.	2.6	6
54	Dynamics of conformational defects in poly(3-hexyl)thiophene. <i>Physical Review B</i> , 1996, 53, 7222-7226.	3.2	5

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55	Investigating charge transport in molecular switches with neural networks. <i>Journal of Computational Chemistry</i> , 1999, 20, 1060-1066.	3.3	5
56	Polaron stability under collision with different defects in conjugated polymers. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2603-2608.	2.0	5
57	Interchain interaction effects on polaronâ€“bipolaron transition on conducting polymers. <i>Journal of Materials Science</i> , 2008, 43, 585-590.	3.7	5
58	Charge Carrier Scattering in Polymers: A New Neutral Coupled Soliton Channel. <i>Scientific Reports</i> , 2018, 8, 6595.	3.3	5
59	Effective Mass of Quasiparticles in Armchair Graphene Nanoribbons. <i>Scientific Reports</i> , 2019, 9, 17990.	3.3	5
60	Charge localization and hopping in a topologically engineered graphene nanoribbon. <i>Scientific Reports</i> , 2021, 11, 5142.	3.3	5
61	Collisions of solitons in polyacetylene. <i>Computational and Theoretical Chemistry</i> , 1997, 394, 161-167.	1.5	4
62	Dynamic interaction between polarons and torsional vibrations in conjugated polymers. <i>International Journal of Quantum Chemistry</i> , 2005, 103, 604-609.	2.0	4
63	Transition of polaron to bipolaron structure in conjugated polymers. <i>Computational and Theoretical Chemistry</i> , 2008, 852, 15-21.	1.5	4
64	Thermal Rate Constant Calculation of the NF + F Reactive System Multiple Arrangements. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8248-8254.	2.5	4
65	Polaron and bipolaron stability on paraphenylene polymers. <i>Journal of Molecular Modeling</i> , 2017, 23, 59.	1.8	4
66	Bipolaron assisted Bloch-like oscillations in organic lattices. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017, 381, 1915-1919.	2.1	4
67	Quasiparticle dynamics by effective π -field distortion. <i>Scientific Reports</i> , 2022, 12, 7967.	3.3	4
68	Linking model Hamiltonians to ab initio and semiempirical methods in descriptions of impurities in conjugated polymers. <i>International Journal of Quantum Chemistry</i> , 2005, 103, 537-542.	2.0	3
69	Effects of impurities on polaron dynamics in conjugated polymers: Effective potentials. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2597-2602.	2.0	3
70	Dynamics of photoexcitations with interchain coupling in conjugated polymers. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2442-2447.	2.0	3
71	Photo-generation of polaron pairs in coupled chains of polyacetylene. <i>Computational and Theoretical Chemistry</i> , 2008, 852, 11-14.	1.5	3
72	A Computational Investigation of the Multiple Channels of the NF ₂ + F Reaction. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14336-14342.	2.5	3

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73	Bloch oscillations in organic and inorganic polymers. <i>Journal of Chemical Physics</i> , 2017, 146, 144903.	3.0	3
74	Dynamical Mechanism of Polarons and Bipolarons in Poly(p-Phenylene Vinylene). <i>Scientific Reports</i> , 2019, 9, 18131.	3.3	3
75	Charge Transport Mechanism in Chevron-Graphene Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2020, 124, 22392-22398.	3.1	3
76	A moving soliton in the TLM model. <i>Synthetic Metals</i> , 1991, 43, 3713-3716.	3.9	2
77	Nonlinear excitations dynamics in molecular switches. <i>Synthetic Metals</i> , 1997, 86, 2245-2246.	3.9	2
78	Interaction of Torsional Oscillations with Polarons and Bipolarons in Conjugated Polymer. <i>Synthetic Metals</i> , 2005, 153, 493-496.	3.9	2
79	Chain length effects on nonlinear excitation transitions in trans- ϵ -polyacetylene. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2507-2511.	2.0	2
80	H_{2^+} dynamical properties in the electronic states $7j\tilde{f}$, $8j\tilde{f}$, $8k\tilde{f}$, $7i\tilde{e}$, and $8j\tilde{p}$. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1316-1320.	2.0	2
81	Influence of bipolaron density on the transport properties of thermalized organic conductors. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2540-2545.	2.0	2
82	Electron-phonon coupling effects on intrachain polaron recombination in conjugated polymers. <i>Journal of Molecular Modeling</i> , 2017, 23, 42.	1.8	2
83	Polaron properties in 2D organic molecular crystals: directional dependence of non-local electron-phonon coupling. <i>Journal of Molecular Modeling</i> , 2019, 25, 149.	1.8	2
84	Quantum bits with polyacetylene. <i>Journal of Computational Chemistry</i> , 2002, 23, 870-873.	3.3	1
85	Polyacetylene as a qubit system. <i>International Journal of Quantum Chemistry</i> , 2003, 95, 224-229.	2.0	1
86	Structural phases of coupled polyacetylene chains with impurities. <i>International Journal of Quantum Chemistry</i> , 2005, 103, 597-603.	2.0	1
87	Quantum-controlled NOT gate made of coupled polyacetylene chains. <i>International Journal of Quantum Chemistry</i> , 2005, 103, 543-549.	2.0	1
88	An extensive investigation of reactions involved in the nitrogen trifluoride dissociation. <i>New Journal of Chemistry</i> , 2013, 37, 3244.	2.8	1
89	Dynamic Formation of Bipolaron-Exciton Complexes in Conducting Polymers. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3866-3872.	2.5	1
90	Structure of the Moving Soliton in the TLM Model. <i>Journal of the Physical Society of Japan</i> , 1993, 62, 2745-2756.	1.6	0

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91	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
92	Dynamics Simulation of Conducting Polymer Interchain Interaction Effects on Polaron Transition. Lecture Notes in Computer Science, 2007, , 304-311.	1.3	0
93	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