

Pedro Henrique de Oliveira Neto

List of Publications by Year in descending order

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papers

567
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567281

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docs citations

53
times ranked

393
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	Electron-Lattice Coupling in Armchair Graphene Nanoribbons. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3039-3042.	4.6	41
3	Improving the Description of the Optical Properties of Carotenoids by Tuning the Long-Range Corrected Functionals. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4944-4950.	2.5	32
4	Intramolecular reorganization energy in zinc phthalocyanine and its fluorinated derivatives: a joint experimental and theoretical study. <i>Chemical Communications</i> , 2013, 49, 6069.	4.1	24
5	Thermal effects on photogeneration of free carriers in organic conductors. <i>Chemical Physics Letters</i> , 2010, 493, 283-287.	2.6	22
6	Dynamics of charge carriers on hexagonal nanoribbons with vacancy defects. <i>Physical Review B</i> , 2016, 94, .	3.2	21
7	Polaron Properties in Armchair Graphene Nanoribbons. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4893-4900.	2.5	21
8	Impurity effects and temperature influence on the exciton dissociation dynamics in conjugated polymers. <i>Chemical Physics Letters</i> , 2013, 580, 108-114.	2.6	20
9	Vibrational and Electronic Structure Analysis of a Carbon Dioxide Interaction with Functionalized Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2854-2861.	2.5	20
10	Dynamical Study of Impurity Effects on Bipolaron-Bipolaron and Bipolaron-Polaron Scattering in Conjugated Polymers. <i>Journal of Physical Chemistry B</i> , 2013, 117, 11801-11811.	2.6	20
11	Charge carrier untrapping by temperature effects in conjugated polymers. <i>Europhysics Letters</i> , 2009, 88, 67006.	2.0	18
12	Impurity effects on polaron-exciton formation in conjugated polymers. <i>Journal of Chemical Physics</i> , 2013, 139, 174903.	3.0	18
13	Dynamics of charge quasiparticles generation in armchair graphene nanoribbons. <i>Carbon</i> , 2018, 132, 352-358.	10.3	16
14	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
15	Predicting the equilibrium structure of organic semiconductors with genetic algorithms. <i>Chemical Physics Letters</i> , 2013, 555, 168-172.	2.6	15
16	Ultrafast direct generation of quasiparticles in graphene nanoribbons. <i>Carbon</i> , 2020, 158, 553-558.	10.3	15
17	Kinetic Monte Carlo model for the COVID-19 epidemic: Impact of mobility restriction on a COVID-19 outbreak. <i>Physical Review E</i> , 2020, 102, 032133.	2.1	15
18	Fast predictions of exciton diffusion length in organic materials. <i>Journal of Materials Chemistry C</i> , 2019, 7, 4066-4071.	5.5	13

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19	Temperature effects on polaron stability in polyacetylene. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2448-2453.	2.0	12
20	Limit of Exciton Diffusion in Highly Ordered π -Conjugated Systems. <i>Journal of Physical Chemistry C</i> , 2015, 119, 19654-19659.	3.1	10
21	Smooth gap tuning strategy for cove-type graphene nanoribbons. <i>RSC Advances</i> , 2020, 10, 26937-26943.	3.6	10
22	Bond length pattern associated with charge carriers in armchair graphene nanoribbons. <i>Journal of Molecular Modeling</i> , 2017, 23, 293.	1.8	9
23	Exciton Diffusion in Organic Nanofibers: A Monte Carlo Study on the Effects of Temperature and Dimensionality. <i>Scientific Reports</i> , 2018, 8, 14066.	3.3	9
24	Modeling temperature dependent singlet exciton dynamics in multilayered organic nanofibers. <i>Journal of Chemical Physics</i> , 2018, 148, 204101.	3.0	8
25	Role of Exciton Density in Organic Materials: Diffusion Length, Lifetime, and Quantum Efficiency. <i>Chemistry of Materials</i> , 2019, 31, 6818-6823.	6.7	8
26	Quasiparticle description of transition metal dichalcogenide nanoribbons. <i>Physical Review B</i> , 2019, 99, .	3.2	8
27	Charge transport in cove-type graphene nanoribbons: The role of quasiparticles. <i>Synthetic Metals</i> , 2022, 287, 117056.	3.9	8
28	Supersonic quasi-particles dynamics in organic semiconductors. <i>Chemical Physics Letters</i> , 2012, 550, 146-149.	2.6	7
29	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
30	Trap-assisted charge transport at conjugated polymer interfaces. <i>Chemical Physics Letters</i> , 2016, 644, 121-126.	2.6	7
31	Triplet-to-singlet exciton transfer in hyperfluorescent OLED materials. <i>Journal of Materials Chemistry C</i> , 2022, 10, 4914-4922.	5.5	7
32	Biexciton cascade emission in multilayered organic nanofibers. <i>Applied Physics Letters</i> , 2018, 112, 143301.	3.3	6
33	Concentration effects on the thermally-activated transport of polarons in conducting polymers. <i>Chemical Physics Letters</i> , 2019, 716, 162-166.	2.6	6
34	Theoretical Investigation on H ₂ O ₂ -Ng (He, Ne, Ar, Kr, Xe, and Rn) Complexes Suitable for Stereodynamics: Interactions and Thermal Chiral Rate Consequences. <i>Frontiers in Chemistry</i> , 2019, 6, 671.	3.6	5
35	Effective Mass of Quasiparticles in Armchair Graphene Nanoribbons. <i>Scientific Reports</i> , 2019, 9, 17990.	3.3	5
36	Charge localization and hopping in a topologically engineered graphene nanoribbon. <i>Scientific Reports</i> , 2021, 11, 5142.	3.3	5

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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	Activation Energies and Diffusion Coefficients of Polarons and Bipolarons in Organic Conductors. Journal of Physical Chemistry A, 2018, 122, 5925-5930.	2.5	4
39	Assessing the effects of increasing conjugation length on exciton diffusion: from small molecules to the polymeric limit. Physical Chemistry Chemical Physics, 2021, 23, 15635-15644.	2.8	4
40	Quasiparticle dynamics by effective π -field distortion. Scientific Reports, 2022, 12, 7967.	3.3	4
41	Dynamics of photoexcitations with interchain coupling in conjugated polymers. International Journal of Quantum Chemistry, 2008, 108, 2442-2447.	2.0	3
42	Photo-generation of polaron pairs in coupled chains of polyacetylene. Computational and Theoretical Chemistry, 2008, 852, 11-14.	1.5	3
43	Dynamical Mechanism of Polarons and Bipolarons in Poly(p-Phenylene Vinylene). Scientific Reports, 2019, 9, 18131.	3.3	3
44	A Genetic Algorithm Approach to Design Principles for Organic Photovoltaic Materials. Advanced Theory and Simulations, 2020, 3, 2000042.	2.8	3
45	Chain length effects on nonlinear excitation transitions in trans-polyacetylene. International Journal of Quantum Chemistry, 2008, 108, 2507-2511.	2.0	2
46	Influence of bipolaron density on the transport properties of thermalized organic conductors. International Journal of Quantum Chemistry, 2013, 113, 2540-2545.	2.0	2
47	Choice of Solubilizing Group Is Determinant for Exciton Diffusion Length in Organic Crystals. Journal of Physical Chemistry C, 2020, 124, 5522-5527.	3.1	2
48	An extensive investigation of reactions involved in the nitrogen trifluoride dissociation. New Journal of Chemistry, 2013, 37, 3244.	2.8	1
49	Dynamical exciton decay in organic materials: the role of bimolecular recombination. Physical Chemistry Chemical Physics, 2019, 21, 1711-1716.	2.8	1
50	Electronic structure of vertically coupled double quantum dots: Optimization of basis functions. Chemical Physics Letters, 2010, 494, 228-231.	2.6	0
51	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
52	Charge-transport in Organic Semiconductors: Probing High Mobility with Light. Materials Research Society Symposia Proceedings, 2013, 1568, 1.	0.1	0
53	Torsional Fracture of Carbon Nanotube Bundles: A Reactive Molecular Dynamics Study. Physical Chemistry Chemical Physics, 0, , .	2.8	0