Luiz A Ribeiro

List of Publications by Year
in descending order

101 papers	899 citations	567247 15 h-index	642715 23 g-index
101 all docs	101 docs citations	101 times ranked	534 citing authors

#	Article	IF	Citations
1	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
2	Transport of Polarons in Graphene Nanoribbons. Journal of Physical Chemistry Letters, 2015, 6, 510-514.	4.6	41
3	Polaron stability in molecular semiconductors: theoretical insight into the impact of the temperature, electric field and the system dimensionality. Physical Chemistry Chemical Physics, 2015, 17, 8973-8982.	2.8	36
4	Exciton dissociation and charge carrier recombination processes in organic semiconductors. Journal of Chemical Physics, 2011, 135, 224901.	3.0	34
5	Critical temperature and products of intrachain polaron recombination in conjugated polymers. Physical Chemistry Chemical Physics, 2014, 16, 17072-17080.	2.8	34
6	Impurity effects on polaron dynamics in graphene nanoribbons. Carbon, 2015, 91, 171-177.	10.3	26
7	On the Mechanical Properties and Thermal Stability of a Recently Synthesized Monolayer Amorphous Carbon. Journal of Physical Chemistry C, 2020, 124, 14855-14860.	3.1	25
8	Kinetics of the OH+HClâ†'H₂O+Cl reaction: Rate determining roles of stereodynamics and roaming and of quantum tunneling. Journal of Computational Chemistry, 2018, 39, 2508-2516.	3.3	22
9	Impact of the electronâ€“phonon coupling symmetry on the polaron stability and mobility in organic molecular semiconductors. Physical Chemistry Chemical Physics, 2016, 18, 1386-1391.	2.8	21
10	Impurity effects and temperature influence on the exciton dissociation dynamics in conjugated polymers. Chemical Physics Letters, 2013, 580, 108-114.	2.6	20
11	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
12	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
13	Impurity effects on polaron-exciton formation in conjugated polymers. Journal of Chemical Physics, 2013, 139, 174903.	3.0	18
14	Predicting the equilibrium structure of organic semiconductors with genetic algorithms. Chemical Physics Letters, 2013, 555, 168-172.	2.6	15
15	Influence of quasi-particle density over polaron mobility in armchair graphene nanoribbons. Physical Chemistry Chemical Physics, 2018, 20, 16712-16718.	2.8	15
16	Ultrafast direct generation of quasiparticles in graphene nanoribbons. Carbon, 2020, 158, 553-558.	10.3	15
17	Tuning Penta-Graphene Electronic Properties Through Engineered Line Defects. Scientific Reports, 2020, 10, 8014.	3.3	15
18	Dynamics of Photogenerated Polaron-Excitons in Organic Semiconductors. Physics Procedia, 2012, 28, 112-116.	1.2	14

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19	A DFT study of a set of natural dyes for organic electronics. Journal of Molecular Modeling, 2017, 23, 343.	1.8	14
20	Bipolaron Dynamics in Graphene Nanoribbons. Scientific Reports, 2019, 9, 2909.	3.3	14
21	On the mechanical properties and fracture patterns of the nonbenzenoid carbon allotrope (biphenylene network): a reactive molecular dynamics study. Nanoscale, 2022, 14, 3200-3211.	5.6	14
22	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
23	Reactive Scattering between Excitons and Charge Carriers in Conjugated Polymers. Journal of Physical Chemistry C, 2014, 118, 23451-23458.	3.1	13
24	Temperature effects on intrachain recombination of bipolarons in conjugated polymers. Chemical Physics Letters, 2014, 614, 151-155.	2.6	12
25	Optimally tuned functionals improving the description of optical and electronic properties of the phthalocyanine molecule. Journal of Molecular Modeling, 2017, 23, 71.	1.8	12
26	O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e362" altimg="si73.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math>adsorption on defective Penta-Graphene lattices: A DFT study. Chemical Physics Letters, 2021, 763, 138229.	2.6	12
27	Temperature Effects on the Scattering of Polarons and Bipolarons in Organic Conductors. Journal of Physical Chemistry A, 2014, 118, 6272-6277.	2.5	11
28	Modeling the Emission Spectra of Organic Molecules: A Competition between Franckâ€“Condon and Nuclear Ensemble Methods. Journal of Physical Chemistry A, 2016, 120, 5380-5388.	2.5	11
29	Polaron dynamics in anisotropic Holsteinâ€“Peierls systems. Physical Chemistry Chemical Physics, 2017, 19, 4078-4084.	2.8	11
30	Electronic couplings and rates of excited state charge transfer processes at poly(thiophene-co-quinoxaline)â€“PC₇₁BM interfaces: two- versus multi-state treatments. Physical Chemistry Chemical Physics, 2019, 21, 25606-25625.	2.8	11
31	Encapsulated Î²-carotene in ZnO nanotubes: Theoretical insight into the stabilization dynamics. Chemical Physics Letters, 2015, 636, 62-66.	2.6	10
32	Tuning the electronic structure properties of MoS₂ monolayers with carbon doping. Physical Chemistry Chemical Physics, 2019, 21, 11168-11174.	2.8	10
33	Bond length pattern associated with charge carriers in armchair graphene nanoribbons. Journal of Molecular Modeling, 2017, 23, 293.	1.8	9
34	Stationary polaron properties in organic crystalline semiconductors. Physical Chemistry Chemical Physics, 2019, 21, 2727-2733.	2.8	9
35	Modeling Polaron Diffusion in Oligoacene-like Crystals. Journal of Physical Chemistry C, 2019, 123, 4715-4720.	3.1	9
36	Adsorption of carbon dioxide and ammonia in transition metalâ€“doped boron nitride nanotubes. Journal of Molecular Modeling, 2019, 25, 359.	1.8	9

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37	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
38	Spin-Orbit Effects on the Dynamical Properties of Polarons in Graphene Nanoribbons. Scientific Reports, 2018, 8, 1914.	3.3	8
39	Role of Exciton Density in Organic Materials: Diffusion Length, Lifetime, and Quantum Efficiency. Chemistry of Materials, 2019, 31, 6818-6823.	6.7	8
40	Stability conditions of armchair graphene nanoribbon bipolarons. Journal of Molecular Modeling, 2019, 25, 245.	1.8	8
41	Electronic structure properties of transition metal dichalcogenide nanotubes: a DFT benchmark. Journal of Molecular Modeling, 2019, 25, 290.	1.8	8
42	Quasiparticle description of transition metal dichalcogenide nanoribbons. Physical Review B, 2019, 99, .	3.2	8
43	Transport of quasiparticles in coronene-based graphene nanoribbons. Journal of Materials Chemistry C, 2020, 8, 12100-12107.	5.5	8
44	A reactive molecular dynamics study on the mechanical properties of a recently synthesized amorphous carbon monolayer converted into a nanotube/nanoscroll. Physical Chemistry Chemical Physics, 2021, 23, 9089-9095.	2.8	8
45	Charge transport in cove-type graphene nanoribbons: The role of quasiparticles. Synthetic Metals, 2022, 287, 117056.	3.9	8
46	Concentration effects on intrachain polaron recombination in conjugated polymers. Physical Chemistry Chemical Physics, 2015, 17, 1299-1308.	2.8	7
47	Trap-assisted charge transport at conjugated polymer interfaces. Chemical Physics Letters, 2016, 644, 121-126.	2.6	7
48	Stationary and Dynamical Properties of Polarons in Anisotropic C₆₀-Crystals. Journal of Physical Chemistry C, 2019, 123, 13410-13418.	3.1	7
49	Electronic and structural properties of vacancy endowed BCN heterostructures. Chemical Physics Letters, 2019, 724, 103-109.	2.6	7
50	On the Elastic Properties and Fracture Patterns of MoX2 (X = S, Se, Te) Membranes: A Reactive Molecular Dynamics Study. Condensed Matter, 2020, 5, 73.	1.8	7
51	Tuning magnetic properties of penta-graphene bilayers through doping with boron, nitrogen, and oxygen. Scientific Reports, 2020, 10, 16748.	3.3	7
52	Optoelectronic properties of amorphous carbon-based nanotube and nanoscroll. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 130, 114683.	2.7	7
53	Defective graphene domains in boron nitride sheets. Journal of Molecular Modeling, 2019, 25, 230.	1.8	6
54	Concentration effects on the thermally-activated transport of polarons in conducting polymers. Chemical Physics Letters, 2019, 716, 162-166.	2.6	6

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55	On the elastic properties of single-walled phagraphene nanotubes. Chemical Physics Letters, 2020, 756, 137830.	2.6	6
56	On the adsorption mechanism of caffeine on MAPbI₃ perovskite surfaces: a combined UMC-DFT study. Physical Chemistry Chemical Physics, 2021, 23, 10807-10813.	2.8	6
57	Nonadiabatic dynamics of injected holes in conjugated polymers. Physical Chemistry Chemical Physics, 2017, 19, 10000-10008.	2.8	5
58	Charge Carrier Scattering in Polymers: A New Neutral Coupled Soliton Channel. Scientific Reports, 2018, 8, 6595.	3.3	5
59	Polaron properties in pentathienoacene crystals. Synthetic Metals, 2019, 253, 34-39.	3.9	5
60	Effective Mass of Quasiparticles in Armchair Graphene Nanoribbons. Scientific Reports, 2019, 9, 17990.	3.3	5
61	Temperature Effects on the Fracture Dynamics and Elastic Properties of Popgraphene Membranes. ChemPhysChem, 2020, 21, 1918-1924.	2.1	5
62	Thermomechanical insight into the stability of nanoporous graphene membranes. FlatChem, 2020, 24, 100196.	5.6	5
63	Charge localization and hopping in a topologically engineered graphene nanoribbon. Scientific Reports, 2021, 11, 5142.	3.3	5
64	Dynamics and structural transformations of carbon onion-like structures under high-velocity impacts. Carbon, 2022, 189, 422-429.	10.3	5
65	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
66	Polaron dynamics in oligoacene stacks. Journal of Molecular Modeling, 2017, 23, 257.	1.8	4
67	Krypton-methanol spectroscopic study: Assessment of the complexation dynamics and the role of the van der Waals interaction. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 205, 179-185.	3.9	4
68	Structural and electronic properties of defective AlN/GaN hybrid nanostructures. Computational Materials Science, 2020, 183, 109860.	3.0	4
69	Electronic and structural properties of Janus MoSSe/MoX2 (XÂ=ÂS,Se) in-plane heterojunctions: A DFT study. Chemical Physics Letters, 2021, 771, 138495.	2.6	4
70	Polaron stability in oligoacene crystals. Journal of Molecular Modeling, 2017, 23, 89.	1.8	3
71	Bloch oscillations in organic and inorganic polymers. Journal of Chemical Physics, 2017, 146, 144903.	3.0	3
72	Combined UMCâ€" DFT prediction of electron-hole coupling in unit cells of pentacene crystals. Journal of Molecular Modeling, 2017, 23, 153.	1.8	3

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73	On the Angular Distribution of the H+Li2 Cross Sections: a Converged Time-Independent Quantum Scattering Study. Scientific Reports, 2018, 8, 1044.	3.3	3
74	Dynamical Mechanism of Polarons and Bipolarons in Poly(p-Phenylene Vinylene). Scientific Reports, 2019, 9, 18131.	3.3	3
75	Charge Transport Mechanism in Chevron-Graphene Nanoribbons. Journal of Physical Chemistry C, 2020, 124, 22392-22398.	3.1	3
76	SimulaÃ§Ã£o de experimentos histÃ³ricos no ensino de fÃsica: uma abordagem computacional das dimensÃµes histÃ³rica e empÃrica da ciÃªncia na sala de aula. Revista Brasileira De Ensino De Fisica, 2012, 34, .	0.2	3
77	Electronâ€“phonon coupling effects on intrachain polaron recombination in conjugated polymers. Journal of Molecular Modeling, 2017, 23, 42.	1.8	2
78	Optical and electronic structure description of metal-doped phthalocyanines. Journal of Molecular Modeling, 2017, 23, 172.	1.8	2
79	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
80	Polaron Diffusion in Pentathienoacene Crystals. Scientific Reports, 2020, 10, 7665.	3.3	2
81	Self-folding and self-scrolling mechanisms of edge-deformed graphene sheets: a molecular dynamics study. Physical Chemistry Chemical Physics, 2021, 23, 15313-15318.	2.8	2
82	Predicting the energetic stabilization of Janus-MoSSe/AlN heterostructures: A DFT study. Chemical Physics Letters, 2021, 771, 138465.	2.6	2
83	Polaron transport in porous graphene nanoribbons. Computational Materials Science, 2021, 194, 110423.	3.0	2
84	A DFT study on the electronic structure of in-plane heterojunctions of graphene and hexagonal boron nitride nanoribbons. Electronic Structure, 2021, 3, 024005.	2.8	2
85	Inferring changes in Ï€-stack mobility induced by aging from vibronic transitions in poly(3-hexylthiophene-2,5-diyl) films. Synthetic Metals, 2019, 247, 276-284.	3.9	2
86	On the Stabilization of Carbynes Encapsulated in Penta-Graphene Nanotubes: a DFT Study. Journal of Molecular Modeling, 2021, 27, 318.	1.8	2
87	Experimental and theoretical description of the optical properties of Myrcia sylvatica essential oil. Journal of Molecular Modeling, 2017, 23, 196.	1.8	2
88	Outcome of sex determination from ulnar and radial ridge densities of Brazilians' fingerprints: Applying an existing method to a new population. Science and Justice - Journal of the Forensic Science Society, 2022, 62, 181-192.	2.1	2
89	Optical properties of P3HT and N2200 polymers: a performance study of an optimally tuned DFT functional. Journal of Molecular Modeling, 2018, 24, 32.	1.8	1
90	Dynamic Formation of Bipolaronâ€“Exciton Complexes in Conducting Polymers. Journal of Physical Chemistry A, 2018, 122, 3866-3872.	2.5	1

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91	Dynamical exciton decay in organic materials: the role of bimolecular recombination. Physical Chemistry Chemical Physics, 2019, 21, 1711-1716.	2.8	1
92	Bloch Oscillations in Fibonacci lattices: polaron formation. Journal of Molecular Modeling, 2019, 25, 102.	1.8	1
93	Bosonic Charge Carriers in Necklace-like Graphene Nanoribbons. Journal of Physical Chemistry Letters, 2020, 11, 5538-5543.	4.6	1
94	On the electronic structure of a recently synthesized graphene-like BCN monolayer from bis-BN cyclohexane with single-atom vacancies: a DFT study. Electronic Structure, 2021, 3, 014006.	2.8	1
95	Intrinsic properties of bipolarons in armchair graphene nanoribbons. Chemical Physics Letters, 2021, 769, 138387.	2.6	1
96	Modeling optical properties of polymerâ€“solvent complexes: the chloroform influence on the P3HT and N2200 absorption spectra. Journal of Molecular Modeling, 2017, 23, 37.	1.8	0
97	Polaron formation at impurity-endowed lattices. Journal of Molecular Modeling, 2019, 25, 95.	1.8	0
98	Theoretical prediction of electron mobility in birhodanine crystals and their sulfur analogs. Chemical Physics Letters, 2021, 763, 138226.	2.6	0
99	Organic Electronics from Nature: Computational Investigation of the Electronic and Optical Properties of the Isomers of Bixin and Norbixin Present in the Achiote Seeds. Molecules, 2022, 27, 2138.	3.8	0
100	DeterminaÃ§Ã£o do sexo a partir da densidade de linhas distal e proximal das impressÃµes digitais de brasileiros. Research, Society and Development, 2022, 11, e7311528057.	0.1	0
101	Torsional Fracture of Carbon Nanotube Bundles: A Reactive Molecular Dynamics Study. Physical Chemistry Chemical Physics, 0, , .	2.8	0