Luiz A Ribeiro

List of Publications by Citations

96 papers	655 citations	14 h-index	20 g-index
101 ext. papers	755 ext. citations	3.4 avg, IF	4.45 L-index

#	Paper	IF	Citations
96	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
95	Transport of Polarons in Graphene Nanoribbons. *Journal of Physical Chemistry Letters*, **2015**, 6, 510-4	6.4	36
94	Critical temperature and products of intrachain polaron recombination in conjugated polymers. *Physical Chemistry Chemical Physics*, **2014**, 16, 17072-80	3.6	33
93	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, 8973-82	3.6	30
92	Exciton dissociation and charge carrier recombination processes in organic semiconductors. *Journal of Chemical Physics*, **2011**, 135, 224901	3.9	30
91	Impurity effects on polaron dynamics in graphene nanoribbons. *Carbon*, **2015**, 91, 171-177	10.4	24
90	Impurity effects and temperature influence on the exciton dissociation dynamics in conjugated polymers. *Chemical Physics Letters*, **2013**, 580, 108-114	2.5	19
89	Impurity effects on polaron-exciton formation in conjugated polymers. *Journal of Chemical Physics*, **2013**, 139, 174903	3.9	18
88	Impact of the electron-phonon coupling symmetry on the polaron stability and mobility in organic molecular semiconductors. *Physical Chemistry Chemical Physics*, **2016**, 18, 1386-91	3.6	17
87	Dynamical study of impurity effects on bipolaron-bipolaron and bipolaron-polaron scattering in conjugated polymers. *Journal of Physical Chemistry B*, **2013**, 117, 11801-11	3.4	17
86	Impact of the Electron-Phonon Interactions on the Polaron Dynamics in Graphene Nanoribbons. *Journal of Physical Chemistry A*, **2016**, 120, 4901-6	2.8	16
85	Predicting the equilibrium structure of organic semiconductors with genetic algorithms. *Chemical Physics Letters*, **2013**, 555, 168-172	2.5	15
84	Kinetics of the OH+HCl-þ O+Cl reaction: Rate determining roles of stereodynamics and roaming and of quantum tunneling. *Journal of Computational Chemistry*, **2018**, 39, 2508-2516	3.5	15
83	Dynamics of Photogenerated Polaron-Excitons in Organic Semiconductors. *Physics Procedia*, **2012**, 28, 112-116		14
82	Influence of quasi-particle density over polaron mobility in armchair graphene nanoribbons. *Physical Chemistry Chemical Physics*, **2018**, 20, 16712-16718	3.6	14
81	Reactive Scattering between Excitons and Charge Carriers in Conjugated Polymers. *Journal of Physical Chemistry C*, **2014**, 118, 23451-23458	3.8	12
80	A DFT study of a set of natural dyes for organic electronics. *Journal of Molecular Modeling*, **2017**, 23, 3432		12

79	Ultrafast direct generation of quasiparticles in graphene nanoribbons. *Carbon*, **2020**, 158, 553-558	10.4	12
78	Bipolaron Dynamics in Graphene Nanoribbons. *Scientific Reports*, **2019**, 9, 2909	4.9	12
77	Temperature effects on intrachain recombination of bipolarons in conjugated polymers. *Chemical Physics Letters*, **2014**, 614, 151-155	2.5	11
76	Spectroscopic properties of the molecular ion in the 8k□9k□9l□9l□and 10o□electronic states. *Journal of Molecular Spectroscopy*, **2012**, 273, 26-29	1.3	11
75	Optimally tuned functionals improving the description of optical and electronic properties of the phthalocyanine molecule. *Journal of Molecular Modeling*, **2017**, 23, 71	2	10
74	Polaron dynamics in anisotropic Holstein-Peierls systems. *Physical Chemistry Chemical Physics*, **2017**, 19, 4078-4084	3.6	9
73	Temperature effects on the scattering of polarons and bipolarons in organic conductors. *Journal of Physical Chemistry A*, **2014**, 118, 6272-7	2.8	9
72	Modeling the Emission Spectra of Organic Molecules: A Competition between Franck-Condon and Nuclear Ensemble Methods. *Journal of Physical Chemistry A*, **2016**, 120, 5380-8	2.8	9
71	Bond length pattern associated with charge carriers in armchair graphene nanoribbons. *Journal of Molecular Modeling*, **2017**, 23, 293	2	8
70	Tuning the electronic structure properties of MoS monolayers with carbon doping. *Physical Chemistry Chemical Physics*, **2019**, 21, 11168-11174	3.6	7
69	On the Mechanical Properties and Thermal Stability of a Recently Synthesized Monolayer Amorphous Carbon. *Journal of Physical Chemistry C*, **2020**, 124, 14855-14860	3.8	7
68	Spin-Orbit Effects on the Dynamical Properties of Polarons in Graphene Nanoribbons. *Scientific Reports*, **2018**, 8, 1914	4.9	7
67	Stability conditions of armchair graphene nanoribbon bipolarons. *Journal of Molecular Modeling*, **2019**, 25, 245	2	7
66	Singlet-singlet exciton recombination: theoretical insight into the influence of high density regime of excitons in conjugated polymers. *Journal of Physical Chemistry B*, **2014**, 118, 5250-7	3.4	7
65	Quasiparticle description of transition metal dichalcogenide nanoribbons. *Physical Review B*, **2019**, 99,	3.3	7
64	Stationary polaron properties in organic crystalline semiconductors. *Physical Chemistry Chemical Physics*, **2019**, 21, 2727-2733	3.6	6
63	Electronic and structural properties of vacancy endowed BCN heterostructures. *Chemical Physics Letters*, **2019**, 724, 103-109	2.5	6
62	Concentration effects on intrachain polaron recombination in conjugated polymers. *Physical Chemistry Chemical Physics*, **2015**, 17, 1299-308	3.6	6

61	Encapsulated Ecarotene in ZnO nanotubes: Theoretical insight into the stabilization dynamics. *Chemical Physics Letters*, **2015**, 636, 62-66	2.5	6
60	Role of Exciton Density in Organic Materials: Diffusion Length, Lifetime, and Quantum Efficiency. *Chemistry of Materials*, **2019**, 31, 6818-6823	9.6	6
59	Nonadiabatic dynamics of injected holes in conjugated polymers. *Physical Chemistry Chemical Physics*, **2017**, 19, 10000-10008	3.6	5
58	Electronic structure properties of transition metal dichalcogenide nanotubes: a DFT benchmark. *Journal of Molecular Modeling*, **2019**, 25, 290	2	5
57	Polaron properties in pentathienoacene crystals. *Synthetic Metals*, **2019**, 253, 34-39	3.6	5
56	Transport of quasiparticles in coronene-based graphene nanoribbons. *Journal of Materials Chemistry C*, **2020**, 8, 12100-12107	7.1	5
55	Trap-assisted charge transport at conjugated polymer interfaces. *Chemical Physics Letters*, **2016**, 644, 121-126	2.5	5
54	Defective graphene domains in boron nitride sheets. *Journal of Molecular Modeling*, **2019**, 25, 230	2	5
53	Tuning Penta-Graphene Electronic Properties Through Engineered Line Defects. *Scientific Reports*, **2020**, 10, 8014	4.9	5
52	Modeling Polaron Diffusion in Oligoacene-like Crystals. *Journal of Physical Chemistry C*, **2019**, 123, 4715-4720	3.8	5
51	Concentration effects on the thermally-activated transport of polarons in conducting polymers. *Chemical Physics Letters*, **2019**, 716, 162-166	2.5	5
50	Stationary and Dynamical Properties of Polarons in Anisotropic C60-Crystals. *Journal of Physical Chemistry C*, **2019**, 123, 13410-13418	3.8	4
49	Polaron dynamics in oligoacene stacks. *Journal of Molecular Modeling*, **2017**, 23, 257	2	4
48	Tuning magnetic properties of penta-graphene bilayers through doping with boron, nitrogen, and oxygen. *Scientific Reports*, **2020**, 10, 16748	4.9	4
47	Effective Mass of Quasiparticles in Armchair Graphene Nanoribbons. *Scientific Reports*, **2019**, 9, 17990	4.9	4
46	Electronic couplings and rates of excited state charge transfer processes at poly(thiophene-co-quinoxaline)-PCBM interfaces: two- versus multi-state treatments. *Physical Chemistry Chemical Physics*, **2019**, 21, 25606-25625	3.6	4
45	Polaron stability in oligoacene crystals. *Journal of Molecular Modeling*, **2017**, 23, 89	2	3
44	Combined UMC- DFT prediction of electron-hole coupling in unit cells of pentacene crystals. *Journal of Molecular Modeling*, **2017**, 23, 153	2	3

43	On the Angular Distribution of the H+Li Cross Sections: a Converged Time-Independent Quantum Scattering Study. *Scientific Reports*, **2018**, 8, 1044	4.9	3
42	Charge Carrier Scattering in Polymers: A New Neutral Coupled Soliton Channel. *Scientific Reports*, **2018**, 8, 6595	4.9	3
41	Charge Transport Mechanism in Chevron-Graphene Nanoribbons. *Journal of Physical Chemistry C*, **2020**, 124, 22392-22398	3.8	3
40	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	3
39	Optoelectronic properties of amorphous carbon-based nanotube and nanoscroll. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 130, 114683	3	3
38	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	4.4	3
37	O2 adsorption on defective Penta-Graphene lattices: A DFT study. *Chemical Physics Letters*, **2021**, 763, 138229	2.5	3
36	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	3.6	3
35	Electron-phonon coupling effects on intrachain polaron recombination in conjugated polymers. *Journal of Molecular Modeling*, **2017**, 23, 42	2	2
34	Structural and electronic properties of defective AlN/GaN hybrid nanostructures. *Computational Materials Science*, **2020**, 183, 109860	3.2	2
33	Inferring changes in π-stack mobility induced by aging from vibronic transitions in poly(3-hexylthiophene-2,5-diyl) films. *Synthetic Metals*, **2019**, 247, 276-284	3.6	2
32	Experimental and theoretical description of the optical properties of Myrcia sylvatica essential oil. *Journal of Molecular Modeling*, **2017**, 23, 196	2	2
31	Thermomechanical insight into the stability of nanoporous graphene membranes. *FlatChem*, **2020**, 24, 100196	5.1	2
30	Charge localization and hopping in a topologically engineered graphene nanoribbon. *Scientific Reports*, **2021**, 11, 5142	4.9	2
29	Predicting the energetic stabilization of Janus-MoSSe/AlN heterostructures: A DFT study. *Chemical Physics Letters*, **2021**, 771, 138465	2.5	2
28	Dynamical Mechanism of Polarons and Bipolarons in Poly(p-Phenylene Vinylene). *Scientific Reports*, **2019**, 9, 18131	4.9	2
27	Adsorption of carbon dioxide and ammonia in transition metal-doped boron nitride nanotubes. *Journal of Molecular Modeling*, **2019**, 25, 359	2	2
26	Bipolaron assisted Bloch-like oscillations in organic lattices. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2017**, 381, 1915-1919	2.3	1

25	Bloch oscillations in organic and inorganic polymers. *Journal of Chemical Physics*, **2017**, 146, 144903	3.9	1
24	Optical and electronic structure description of metal-doped phthalocyanines. *Journal of Molecular Modeling*, **2017**, 23, 172	2	1
23	Dynamical exciton decay in organic materials: the role of bimolecular recombination. *Physical Chemistry Chemical Physics*, **2019**, 21, 1711-1716	3.6	1
22	Bloch Oscillations in Fibonacci lattices: polaron formation. *Journal of Molecular Modeling*, **2019**, 25, 102	2	1
21	Polaron Diffusion in Pentathienoacene Crystals. *Scientific Reports*, **2020**, 10, 7665	4.9	1
20	Bosonic Charge Carriers in Necklace-like Graphene Nanoribbons. *Journal of Physical Chemistry Letters*, **2020**, 11, 5538-5543	6.4	1
19	Optical properties of P3HT and N2200 polymers: a performance study of an optimally tuned DFT functional. *Journal of Molecular Modeling*, **2017**, 24, 32	2	1
18	Dynamic Formation of Bipolaron-Exciton Complexes in Conducting Polymers. *Journal of Physical Chemistry A*, **2018**, 122, 3866-3872	2.8	1
17	Polaron properties in 2D organic molecular crystals: directional dependence of non-local electron-phonon coupling. *Journal of Molecular Modeling*, **2019**, 25, 149	2	1
16	On the Stabilization of Carbynes Encapsulated in Penta-Graphene Nanotubes: a DFT Study. *Journal of Molecular Modeling*, **2021**, 27, 318	2	1
15	On the elastic properties of single-walled phagraphene nanotubes. *Chemical Physics Letters*, **2020**, 756, 137830	2.5	1
14	Temperature Effects on the Fracture Dynamics and Elastic Properties of Popgraphene Membranes. *ChemPhysChem*, **2020**, 21, 1918-1924	3.2	1
13	Electronic and structural properties of Janus MoSSe/MoX2 (X = S,Se) in-plane heterojunctions: A DFT study. *Chemical Physics Letters*, **2021**, 771, 138495	2.5	1
12	On the adsorption mechanism of caffeine on MAPbI perovskite surfaces: a combined UMC-DFT study. *Physical Chemistry Chemical Physics*, **2021**, 23, 10807-10813	3.6	1
11	Charge transport in cove-type graphene nanoribbons: The role of quasiparticles. *Synthetic Metals*, **2022**, 287, 117056	3.6	1
10	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	0
9	Dynamics and structural transformations of carbon onion-like structures under high-velocity impacts. *Carbon*, **2022**, 189, 422-429	10.4	0
8	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	2.6	0

7	A DFT study on the electronic structure of in-plane heterojunctions of graphene and hexagonal boron nitride nanoribbons. *Electronic Structure*, **2021**, 3, 024005	2.6	0
6	Modeling optical properties of polymer-solvent complexes: the chloroform influence on the P3HT and N2200 absorption spectra. *Journal of Molecular Modeling*, **2017**, 23, 37	2	
5	Polaron formation at impurity-endowed lattices. *Journal of Molecular Modeling*, **2019**, 25, 95	2	
4	Intrinsic properties of bipolarons in armchair graphene nanoribbons. *Chemical Physics Letters*, **2021**, 769, 138387	2.5	
3	Polaron transport in porous graphene nanoribbons. *Computational Materials Science*, **2021**, 194, 110423	3.2	
2	Theoretical prediction of electron mobility in birhodanine crystals and their sulfur analogs. *Chemical Physics Letters*, **2021**, 763, 138226	2.5	
1	Self-folding and self-scrolling mechanisms of edge-deformed graphene sheets: a molecular dynamics study. *Physical Chemistry Chemical Physics*, **2021**, 23, 15313-15318	3.6	