Demetrio Da Silva Filho

List of Publications by Year in Descending Order

85 papers	10,517 citations	29 h-index	96 g-index
96 ext. papers	11,166 ext. citations	5.9 avg, IF	5.79 L-index

#	Paper	IF	Citations
85	Long-range parameter optimization for a better description of potential energy surfaces using Density Functional Theory.. *Journal of Molecular Modeling*, **2022**, 28, 121	2	0
84	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
83	Charge localization and hopping in a topologically engineered graphene nanoribbon. *Scientific Reports*, **2021**, 11, 5142	4.9	2
82	Interfacial Bulk Properties of Hole-Transporting Materials for Perovskite Solar Cells: Isomeric Triphenylamine-Based Enamines Spiro-OMeTAD. *ACS Applied Materials & Interfaces*, **2021**, 13, 21320-21330	9.5	2
81	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
80	Theoretical prediction of electron mobility in birhodanine crystals and their sulfur analogs. *Chemical Physics Letters*, **2021**, 763, 138226	2.5	
79	. *IEEE Access*, **2021**, 9, 129605-129618	3.5	2
78	Work function difference of naphthyl end-capped oligothiophene in different crystal alignments studied by Kelvin probe force microscopy. *Organic Electronics*, **2021**, 89, 106060	3.5	1
77	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	3.6	1
76	On the Physical Origins of Charge Separation at Donor–Acceptor Interfaces in Organic Solar Cells: Energy Bending versus Energy Disorder. *Advanced Theory and Simulations*, **2020**, 3, 1900230	3.5	6
75	A Genetic Algorithm Approach to Design Principles for Organic Photovoltaic Materials. *Advanced Theory and Simulations*, **2020**, 3, 2000042	3.5	1
74	Kinetic Monte Carlo model for the COVID-19 epidemic: Impact of mobility restriction on a COVID-19 outbreak. *Physical Review E*, **2020**, 102, 032133	2.4	4
73	Dynamical exciton decay in organic materials: the role of bimolecular recombination. *Physical Chemistry Chemical Physics*, **2019**, 21, 1711-1716	3.6	1
72	Fast predictions of exciton diffusion length in organic materials. *Journal of Materials Chemistry C*, **2019**, 7, 4066-4071	7.1	9
71	Role of Exciton Density in Organic Materials: Diffusion Length, Lifetime, and Quantum Efficiency. *Chemistry of Materials*, **2019**, 31, 6818-6823	9.6	6
70	Hemilabile bonding of 1-oxa-4,7-dithiacyclononane in cyclometallated palladium(ii) complexes. *Dalton Transactions*, **2019**, 48, 11520-11535	4.3	1
69	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

68	Biexciton cascade emission in multilayered organic nanofibers. *Applied Physics Letters*, **2018**, 112, 143301	3.4	6
67	Modeling temperature dependent singlet exciton dynamics in multilayered organic nanofibers. *Journal of Chemical Physics*, **2018**, 148, 204101	3.9	7
66	Exciton Diffusion in Organic Nanofibers: A Monte Carlo Study on the Effects of Temperature and Dimensionality. *Scientific Reports*, **2018**, 8, 14066	4.9	8
65	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	
64	Can Fluorenone-Based Compounds Emit in the Blue Region? Impact of the Conjugation Length and the Ground-State Aggregation. *Chemistry of Materials*, **2017**, 29, 1695-1707	9.6	29
63	Optimally tuned functionals improving the description of optical and electronic properties of the phthalocyanine molecule. *Journal of Molecular Modeling*, **2017**, 23, 71	2	10
62	Optical and electronic structure description of metal-doped phthalocyanines. *Journal of Molecular Modeling*, **2017**, 23, 172	2	1
61	Combined UMC- DFT prediction of electron-hole coupling in unit cells of pentacene crystals. *Journal of Molecular Modeling*, **2017**, 23, 153	2	3
60	Mobility field and mobility temperature dependence in PC61BM: A kinetic Monte-Carlo study. *Chemical Physics Letters*, **2017**, 689, 74-81	2.5	7
59	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
58	Modelling charge transport of discotic liquid-crystalline triindoles: the role of peripheral substitution. *Physical Chemistry Chemical Physics*, **2017**, 19, 24202-24208	3.6	7
57	A DFT study of a set of natural dyes for organic electronics. *Journal of Molecular Modeling*, **2017**, 23, 343	2	12
56	A joint theoretical and experimental characterization of two acene-thiophene derivatives. *Journal of Molecular Modeling*, **2017**, 23, 52	2	1
55	Experimental and theoretical description of the optical properties of Myrcia sylvatica essential oil. *Journal of Molecular Modeling*, **2017**, 23, 196	2	2
54	Strong Solvent Effects on the Nonlinear Optical Properties of Z and E Isomers from Azo-Enaminone Derivatives. *Journal of Physical Chemistry C*, **2016**, 120, 17660-17669	3.8	38
53	Improving the Description of the Optical Properties of Carotenoids by Tuning the Long-Range Corrected Functionals. *Journal of Physical Chemistry A*, **2016**, 120, 4944-50	2.8	25
52	Synthesis, Structure, Properties, and Bioimaging of a Fluorescent Nitrogen-Linked Bisbenzothiadiazole. *Journal of Organic Chemistry*, **2016**, 81, 2958-65	4.2	12
51	Low-Temperature Seebeck Coefficients for Polaron-Driven Thermoelectric Effect in Organic Polymers. *Journal of Physical Chemistry A*, **2016**, 120, 4923-7	2.8	7

50	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
49	Efficient Exciton Diffusion and Resonance-Energy Transfer in Multilayered Organic Epitaxial Nanofibers. *Journal of Physical Chemistry C*, **2015**, 119, 15689-15697	3.8	9
48	Limit of Exciton Diffusion in Highly Ordered Conjugated Systems. *Journal of Physical Chemistry C*, **2015**, 119, 19654-19659	3.8	10
47	Structure and Disorder in Squaraine:C60 Organic Solar Cells: A Theoretical Description of Molecular Packing and Electronic Coupling at the Donor/Acceptor Interface. *Advanced Functional Materials*, **2014**, 24, 3790-3798	15.6	38
46	Designed non-symmetrical 4,7-pi-extended-2,1,3-benzothiadiazole derivatives: Synthesis guided by DFT predictions. *Journal of Physical Organic Chemistry*, **2014**, 27, 303-309	2.1	17
45	Interplay of alternative conjugated pathways and steric interactions on the electronic and optical properties of donor/acceptor conjugated polymers. *Journal of Materials Chemistry C*, **2014**, 2, 8873-8879	7.1	22
44	Design, synthesis and application of fluorescent 2,1,3-benzothiadiazole-triazole-linked biologically active lapachone derivatives. *New Journal of Chemistry*, **2014**, 38, 2569	3.6	43
43	Symmetry Lowering in Triindoles: Impact on the Electronic and Photophysical Properties. *Journal of Physical Chemistry C*, **2014**, 118, 5470-5477	3.8	21
42	Investigation of the torsional barrier of EDOT using molecular mechanics and DFT methods. *Journal of Molecular Modeling*, **2014**, 20, 2405	2	2
41	Amplified Spontaneous Emission in Pentathienoacene Dioxides by Direct Optical Pump and by Energy Transfer: Correlation with Photophysical Parameters. *Advanced Optical Materials*, **2013**, 1, 588-599	8.1	9
40	Intramolecular reorganization energy in zinc phthalocyanine and its fluorinated derivatives: a joint experimental and theoretical study. *Chemical Communications*, **2013**, 49, 6069-71	5.8	24
39	Charge-transport in Organic Semiconductors: Probing High Mobility with Light. *Materials Research Society Symposia Proceedings*, **2013**, 1568, 1		
38	Temperature-induced oscillating electric dipole in conjugated systems. *Chemical Physics Letters*, **2012**, 539-540, 214-217	2.5	8
37	Exciton dissociation and charge carrier recombination processes in organic semiconductors. *Journal of Chemical Physics*, **2011**, 135, 224901	3.9	30
36	Tuning the charge-transport parameters of perylene diimide single crystals via end and/or core functionalization: a density functional theory investigation. *Journal of the American Chemical Society*, **2010**, 132, 3375-87	16.4	293
35	Regiochemistry of Poly(3-hexylthiophene): Synthesis and Investigation of a Conducting Polymer. *Journal of Chemical Education*, **2010**, 87, 522-525	2.4	20
34	Theoretical characterization of charge transport in one-dimensional collinear arrays of organic conjugated molecules. *ChemPhysChem*, **2010**, 11, 1062-8	3.2	34
33	Comparison of thiophene-pyrrole oligomers with oligothiophenes: a joint experimental and theoretical investigation of their structural and spectroscopic properties. *Chemistry - A European Journal*, **2010**, 16, 6866-76	4.8	27

32	Influence of intermolecular vibrations on the electronic coupling in organic semiconductors: the case of anthracene and perfluoropentacene. *ChemPhysChem*, **2009**, 10, 2265-73	3.2	69
31	Inside Cover: Influence of Intermolecular Vibrations on the Electronic Coupling in Organic Semiconductors: The Case of Anthracene and Perfluoropentacene (ChemPhysChem 13/2009). *ChemPhysChem*, **2009**, 10, 2158-2158	3.2	
30	Charge transport in oligo phenylene and phenyleneEthiophene nanofibers. *Organic Electronics*, **2009**, 10, 1228-1234	3.5	27
29	Impact of perfluorination on the charge-transport parameters of oligoacene crystals. *Journal of the American Chemical Society*, **2009**, 131, 1502-12	16.4	165
28	Cyclometallated Pt(II) and Pd(II) complexes with a trithiacrown ligand. *Dalton Transactions*, **2008**, 1872-82	4.3	32
27	Modeling Electron and Hole Transport in Fluoroarene-Oligothiopene Semiconductors: Investigation of Geometric and Electronic Structure Properties. *Advanced Functional Materials*, **2008**, 18, 332-340	15.6	104
26	Cooperative CHInteractions in the Crystal Structure of 2,5-Di(3-biphenyl)-1,1-dimethyl-3,4-diphenyl-silole and Its Effect on Its Electronic Properties. *Journal of Physical Chemistry C*, **2007**, 111, 9543-9547	3.8	21
25	Charge transport in organic semiconductors. *Chemical Reviews*, **2007**, 107, 926-52	68.1	3363
24	Hole-vibronic coupling in oligothiophenes: impact of backbone torsional flexibility on relaxation energies. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2007**, 365, 1435-52	3	56
23	Vibronic coupling in the ground and excited states of oligoacene cations. *Journal of Physical Chemistry B*, **2006**, 110, 18904-11	3.4	128
22	Effect of electronic polarization on charge-transport parameters in molecular organic semiconductors. *Journal of the American Chemical Society*, **2006**, 128, 9882-6	16.4	652
21	N- and P-channel transport behavior in thin film transistors based on tricyanovinyl-capped oligothiophenes. *Journal of Physical Chemistry B*, **2006**, 110, 14590-7	3.4	57
20	Synthesis, X-ray, spectroelectrochemical, and theoretical studies of a tricyanovinyl-capped quaterthiophene: A correlation of semiconductor performance with physical properties. *Chemical Physics Letters*, **2006**, 425, 251-256	2.5	6
19	Shallow trap states in pentacene thin films from molecular sliding. *Applied Physics Letters*, **2005**, 86, 152115	3.4	128
18	Transport Properties in the Rubrene Crystal: Electronic Coupling and Vibrational Reorganization Energy. *Advanced Materials*, **2005**, 17, 1072-1076	24	384
17	Introduction to Organic Thin Film Transistors and Design of n-Channel Organic Semiconductors. *Chemistry of Materials*, **2004**, 16, 4436-4451	9.6	1159
16	Charge transport properties in discotic liquid crystals: a quantum-chemical insight into structure-property relationships. *Journal of the American Chemical Society*, **2004**, 126, 3271-9	16.4	432
15	Molecular hosts for triplet emission in light emitting diodes: A quantum-chemical study. *Chemical Physics Letters*, **2004**, 392, 521-528	2.5	48

14	Preparation and characterization of pi-stacking quinodimethane oligothiophenes. Predicting semiconductor behavior and bandwidths from crystal structures and molecular orbital calculations. *Journal of the American Chemical Society*, **2004**, 126, 15295-308	16.4	120
13	Organic Thin Film Transistors Based on N-Alkyl Perylene Diimides: Charge Transport Kinetics as a Function of Gate Voltage and Temperature. *Journal of Physical Chemistry B*, **2004**, 108, 19281-19292	3.4	383
12	Vibronic coupling in the ground and excited states of the naphthalene cation. *Chemical Communications*, **2004**, 1702-3	5.8	29
11	A multimode analysis of the gas-phase photoelectron spectra in oligoacenes. *Journal of Chemical Physics*, **2004**, 120, 7490-6	3.9	152
10	Three-dimensional band structure and bandlike mobility in oligoacene single crystals: A theoretical investigation. *Journal of Chemical Physics*, **2003**, 118, 3764-3774	3.9	344
9	Influence of apolar group structure on the properties of Langmuir monolayers of polyphenyl carboxylic acids. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2002**, 198-200, 141-150	5.1	1
8	Organic semiconductors: a theoretical characterization of the basic parameters governing charge transport. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 5804-9	11.5	1034
7	Hole- and electron-vibrational couplings in oligoacene crystals: intramolecular contributions. *Physical Review Letters*, **2002**, 89, 275503	7.4	359
6	The vibrational reorganization energy in pentacene: molecular influences on charge transport. *Journal of the American Chemical Society*, **2002**, 124, 7918-9	16.4	376
5	Structural Modification Influences the Characteristics of Langmuir Monolayers from Aromatic Carboxylic Acids. *Journal of Colloid and Interface Science*, **2001**, 239, 158-167	9.3	3
4	Quantitative treatment of surface potentials in Langmuir films from aromatic amphiphiles. *Chemical Physics Letters*, **2001**, 337, 11-17	2.5	13
3	Dipole moments in Langmuir monolayers from aromatic carboxylic acids. *Chemical Physics Letters*, **2000**, 326, 39-44	2.5	11
2	Molecular hyperpolarizabilities of retinal derivatives. *Journal of Chemical Physics*, **1999**, 111, 5102-5106	3.9	10
1	A comparative study of the hyperpolarizabilities of solitonic chains. *Synthetic Metals*, **1999**, 102, 1584	3.6	1