Luca Muccioli

List of Publications by Year
in descending order

99 papers	4,439 citations	101384 36 h-index	110170 64 g-index
100 all docs	100 docs citations	100 times ranked	5039 citing authors

#	Article	IF	Citations
1	Temperature-Dependent Structural Phase Transition in Rubrene Single Crystals: The Missing Piece from the Charge Mobility Puzzle?. Journal of Physical Chemistry Letters, 2022, 13, 406-411.	2.1	4
2	Highlighting the processing versatility of a silicon phthalocyanine derivative for organic thin-film transistors. Journal of Materials Chemistry C, 2022, 10, 485-495.	2.7	16
3	Direct Triple Annulations: A Way to Design Large Triazastarphenes with Intertwined Hexagonal Packing. Organic Letters, 2022, 24, 344-348.	2.4	0
4	Silicon Phthalocyanines for n-Type Organic Thin-Film Transistors: Development of Structureâ€“Property Relationships. ACS Applied Electronic Materials, 2021, 3, 325-336.	2.0	27
5	Self-assembling, structure and nonlinear optical properties of fluorescent organic nanoparticles in water. Physical Chemistry Chemical Physics, 2021, 23, 23643-23654.	1.3	9
6	Bidimensional Hâ€Bond Network Promotes Structural Order and Electron Transport in BPyMPMs Molecular Semiconductor. Advanced Theory and Simulations, 2021, 4, 2000302.	1.3	4
7	N-Type Solution-Processed Tin versus Silicon Phthalocyanines: A Comparison of Performance in Organic Thin-Film Transistors and in Organic Photovoltaics. ACS Applied Electronic Materials, 2021, 3, 1873-1885.	2.0	10
8	Peptoids as a Chiral Stationary Phase for Liquid Chromatography: Insights from Molecular Dynamics Simulations. Biomacromolecules, 2021, 22, 2573-2581.	2.6	6
9	Thin-Film Engineering of Solution-Processable n-Type Silicon Phthalocyanines for Organic Thin-Film Transistors. ACS Applied Materials & Interfaces, 2021, 13, 1008-1020.	4.0	29
10	In Silico Ultrafast Nonlinear Spectroscopy Meets Experiments: The Case of Perylene Bisimide Dye. Journal of Chemical Theory and Computation, 2021, 17, 7134-7145.	2.3	6
11	Self-organization of complete organic monolayers via sequential post-deposition annealing. Progress in Organic Coatings, 2020, 138, 105408.	1.9	15
12	Fate of Low-Lying Charge-Transfer Excited States in a Donor:Acceptor Blend with a Large Energy Offset. Journal of Physical Chemistry Letters, 2020, 11, 10219-10226.	2.1	9
13	Orientation dependent molecular electrostatics drives efficient charge generation in homojunction organic solar cells. Nature Communications, 2020, 11, 4617.	5.8	60
14	Surface-Confined Macrocyclization via Dynamic Covalent Chemistry. ACS Nano, 2020, 14, 2956-2965.	7.3	8
15	Atomistic Simulation of Phase Transitions and Charge Mobility for the Organic Semiconductor Ph-BTBT-C10. Chemistry of Materials, 2019, 31, 7092-7103.	3.2	19
16	Highly emissive excitons with reduced exchange energy in thermally activated delayed fluorescent molecules. Nature Communications, 2019, 10, 597.	5.8	253
17	Multiple Charge Transfer States in Donorâ€“Acceptor Heterojunctions with Large Frontier Orbital Energy Offsets. Chemistry of Materials, 2019, 31, 6808-6817.	3.2	20
18	Nonlinear Optical Contrast in Azobenzene-Based Self-Assembled Monolayers. Chemistry of Materials, 2019, 31, 6759-6769.	3.2	25

#	Article	IF	Citations
19	Solution-Processable n-Type Tin Phthalocyanines in Organic Thin Film Transistors and as Ternary Additives in Organic Photovoltaics. ACS Applied Electronic Materials, 2019, 1, 494-504.	2.0	21
20	Impact of structural anisotropy on electro-mechanical response in crystalline organic semiconductors. Journal of Materials Chemistry C, 2019, 7, 4382-4391.	2.7	10
21	Structure and Charge Transport Properties of Cycloparaphenylene Monolayers on Graphite. Advanced Materials Interfaces, 2019, 6, 1801948.	1.9	7
22	Atomistic simulations of charge transport in photoswitchable organic-graphene hybrids. JPhys Materials, 2019, 2, 035001.	1.8	7
23	Ambipolarity and Dimensionality of Charge Transport in Crystalline Group 14 Phthalocyanines: A Computational Study. Journal of Physical Chemistry C, 2018, 122, 2554-2563.	1.5	20
24	Unusual electromechanical response in rubrene single crystals. Materials Horizons, 2018, 5, 41-50.	6.4	28
25	Nâ€doped cycloparaphenylenes: Tuning electronic properties for applications in thermally activated delayed fluorescence. International Journal of Quantum Chemistry, 2018, 118, e25562.	1.0	9
26	Second-order nonlinear optical properties of Stenhouse photoswitches: insights from density functional theory. Physical Chemistry Chemical Physics, 2018, 20, 27658-27667.	1.3	37
27	Pentacene Crystal Growth on Silica and Layer-Dependent Step-Edge Barrier from Atomistic Simulations. Journal of Physical Chemistry Letters, 2018, 9, 6900-6906.	2.1	25
28	Application of Rubrene Air-Gap Transistors as Sensitive MEMS Physical Sensors. ACS Applied Materials & Interfaces, 2018, 10, 41570-41577.	4.0	10
29	A Festschrift in honour of Professor Claudio Zannoni. Liquid Crystals, 2018, 45, 1871-1879.	0.9	0
30	From rod-like to disc-like Gayâ€“Berne biaxial nematics and back. Liquid Crystals, 2018, 45, 2400-2415.	0.9	4
31	Computational Design of Thermally Activated Delayed Fluorescence Materials: The Challenges Ahead. Journal of Physical Chemistry Letters, 2018, 9, 6149-6163.	2.1	121
32	Dynamical Behavior and Second Harmonic Generation Responses in Acido-Triggered Molecular Switches. Journal of Physical Chemistry C, 2018, 122, 26160-26168.	1.5	24
33	Deep-Blue Oxadiazole-Containing Thermally Activated Delayed Fluorescence Emitters for Organic Light-Emitting Diodes. ACS Applied Materials & Interfaces, 2018, 10, 33360-33372.	4.0	67
34	Nonlinear optical responses of self-assembled monolayers functionalized with indolinoâ€“oxazolidine photoswitches. Physical Chemistry Chemical Physics, 2018, 20, 21590-21597.	1.3	14
35	Carbazole-based Ï€-conjugated polyazomethines: Effects of catenation and comonomer insertion on optoelectronic features. Polymer, 2017, 119, 274-284.	1.8	12
36	Predicting the Conditions for Homeotropic Anchoring of Liquid Crystals at a Soft Surface. 4-n-Pentyl-4â€²-cyanobiphenyl on Alkylsilane Self-Assembled Monolayers. ACS Applied Materials & Interfaces, 2017, 9, 11993-12002.	4.0	26

#	Article	IF	Citations
37	Dynamic nature of excited states of donorâ€“acceptor TADF materials for OLEDs: how theory can reveal structureâ€“property relationships. Journal of Materials Chemistry C, 2017, 5, 5718-5729.	2.7	97
38	Energetic fluctuations in amorphous semiconducting polymers: Impact on charge-carrier mobility. Journal of Chemical Physics, 2017, 147, 134904.	1.2	21
39	Molecular-scale shear response of the organic semiconductor <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi></mml:math> -DBDCS (100) surface. Physical Review B, 2017, 96, .	1.1	3
40	Multi-dimensional charge transport in supramolecular helical foldamer assemblies. Chemical Science, 2017, 8, 7251-7257.	3.7	38
41	Pressure sensor based on organic single crystal air-gap transistor. , 2017, , .		1
42	Nature of the singlet and triplet excitations mediating thermally activated delayed fluorescence. Physical Review Materials, 2017, 1, .	0.9	102
43	Electrostatic phenomena in organic semiconductors: fundamentals and implications for photovoltaics. Journal of Physics Condensed Matter, 2016, 28, 433002.	0.7	131
44	Structural Characterization of Alkylsilane and Fluoroalkylsilane Self-Assembled Monolayers on SiO₂ by Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 14652-14662.	1.5	42
45	Charge Separation and Recombination at Polymerâ€“Fullerene Heterojunctions: Delocalization and Hybridization Effects. Journal of Physical Chemistry Letters, 2016, 7, 536-540.	2.1	93
46	Do charges delocalize over multiple molecules in fullerene derivatives?. Journal of Materials Chemistry C, 2016, 4, 3747-3756.	2.7	44
47	From Chiral Islands to Smectic Layers: A Computational Journey Across Sexithiophene Morphologies on C₆₀. Advanced Functional Materials, 2015, 25, 1985-1995.	7.8	32
48	Theoretical Rationalization of the Singletâ€“Triplet Gap in OLEDs Materials: Impact of Charge-Transfer Character. Journal of Chemical Theory and Computation, 2015, 11, 168-177.	2.3	108
49	Bis(arylene-ethynylene)-s-tetrazines: A Promising Family of n-Type Organic Semiconductors?. Journal of Physical Chemistry C, 2015, 119, 18945-18955.	1.5	18
50	Communication: Molecular dynamics and 1H NMR of n-hexane in liquid crystals. Journal of Chemical Physics, 2015, 143, 011103.	1.2	13
51	Cost-Effective Force Field Tailored for Solid-Phase Simulations of OLED Materials. Journal of Chemical Theory and Computation, 2015, 11, 3383-3392.	2.3	17
52	Molecular organization in freely suspended nano-thick 8CB smectic films. An atomistic simulation. Physical Chemistry Chemical Physics, 2015, 17, 26149-26159.	1.3	16
53	Charge separation energetics at organic heterojunctions: on the role of structural and electrostatic disorder. Physical Chemistry Chemical Physics, 2014, 16, 20279-20290.	1.3	67
54	Electronic Polarization in Organic Crystals: A Comparative Study of Induced Dipoles and Intramolecular Charge Redistribution Schemes. Journal of Chemical Theory and Computation, 2014, 10, 4959-4971.	2.3	76

#	Article	IF	Citations
55	Order and Conformation of Biphenyl in Cyanobiphenyl Liquid Crystals: A Combined Atomistic Molecular Dynamics and ¹H NMR Study. ChemPhysChem, 2014, 15, 1356-1367.	1.0	33
56	Charge Dissociation at Interfaces between Discotic Liquid Crystals: The Surprising Role of Column Mismatch. Journal of the American Chemical Society, 2014, 136, 2911-2920.	6.6	55
57	Quinquephenyl: The Simplest Rigidâ€Rodâ€Like Nematic Liquid Crystal, or is it? An Atomistic Simulation. ChemPhysChem, 2014, 15, 1345-1355.	1.0	30
58	Multiscale Modeling of the Electrostatic Impact of Self-Assembled Monolayers used as Gate Dielectric Treatment in Organic Thin-Film Transistors. ACS Applied Materials & Interfaces, 2014, 6, 15372-15378.	4.0	37
59	On the Supramolecular Packing of High Electron Mobility Naphthalene Diimide Copolymers: The Perfect Registry of Asymmetric Branched Alkyl Side Chains. Macromolecules, 2013, 46, 8171-8178.	2.2	44
60	Exploring the Energy Landscape of the Charge Transport Levels in Organic Semiconductors at the Molecular Scale. Accounts of Chemical Research, 2013, 46, 434-443.	7.6	64
61	Predicting the Anchoring of Liquid Crystals at a Solid Surface: 5-Cyanobiphenyl on Cristobalite and Glassy Silica Surfaces of Increasing Roughness. Langmuir, 2013, 29, 8950-8958.	1.6	62
62	An atomistic description of the nematic and smectic phases of 4-n-octyl-4â€² cyanobiphenyl (8CB). Journal of Chemical Physics, 2013, 138, 204901.	1.2	71
63	Energetics of Electronâ€“Hole Separation at P3HT/PCBM Heterojunctions. Journal of Physical Chemistry C, 2013, 117, 12981-12990.	1.5	126
64	Supramolecular Organization of Functional Organic Materials in the Bulk and at Organic/Organic Interfaces: A Modeling and Computer Simulation Approach. Topics in Current Chemistry, 2013, 352, 39-101.	4.0	18
65	Temperature dependence of charge mobility in model discotic liquid crystals. Physical Chemistry Chemical Physics, 2012, 14, 5368.	1.3	16
66	Predicting surface anchoring: molecular organization across a thin film of 5CB liquid crystal on silicon. Chemical Science, 2012, 3, 573-579.	3.7	69
67	Alignment of Small Organic Solutes in a Nematic Solvent: The Effect of Electrostatic Interactions. Journal of Physical Chemistry B, 2012, 116, 3760-3771.	1.2	21
68	Efficient analysis of highly complex nuclear magnetic resonance spectra of flexible solutes in ordered liquids by using molecular dynamics. Journal of Chemical Physics, 2012, 136, 174506.	1.2	17
69	An atomistic simulation of the liquid-crystalline phases of sexithiophene. Journal of Materials Chemistry, 2011, 21, 125-133.	6.7	59
70	Surface Supramolecular Organization of a Terbium(III) Double-Decker Complex on Graphite and its Single Molecule Magnet Behavior. Journal of the American Chemical Society, 2011, 133, 6603-6612.	6.6	189
71	Assemblies of perylene diimide derivatives with melamine into luminescent hydrogels. Chemical Communications, 2011, 47, 11858.	2.2	73
72	Electronic Processes at Organicâ"Organic Interfaces: Insight from Modeling and Implications for Opto-electronic Devices. Chemistry of Materials, 2011, 23, 591-609.	3.2	185

#	Article	IF	Citations
73	Does supramolecular ordering influence exciton transport in conjugated systems? Insight from atomistic simulations. Chemical Science, 2011, 2, 1025.	3.7	28
74	Simulation of Vaporâ€Phase Deposition and Growth of a Pentacene Thin Film on C₆₀ (001). Advanced Materials, 2011, 23, 4532-4536.	11.1	90
75	How Does the Transâ€“Cis Photoisomerization of Azobenzene Take Place in Organic Solvents?. ChemPhysChem, 2010, 11, 1018-1028.	1.0	140
76	Ferroelectric Response and Induced Biaxiality in the Nematic Phase of Bentâ€Core Mesogens. Advanced Functional Materials, 2009, 19, 2592-2600.	7.8	187
77	Modeling Polymer Dielectric/Pentacene Interfaces: On the Role of Electrostatic Energy Disorder on Charge Carrier Mobility. Advanced Functional Materials, 2009, 19, 3254-3261.	7.8	81
78	Towards in Silico Liquid Crystals. Realistic Transition Temperatures and Physical Properties for nâ€Cyanobiphenyls via Molecular Dynamics Simulations. ChemPhysChem, 2009, 10, 125-136.	1.0	166
79	Conformational Preferences of the Full Chicken Prion Protein in Solution and Its Differences with Respect to Mammals. ChemPhysChem, 2009, 10, 1500-1510.	1.0	8
80	Theoretical Characterization of the Structural and Hole Transport Dynamics in Liquid-Crystalline Phthalocyanine Stacks. Journal of Physical Chemistry B, 2009, 113, 14102-14111.	1.2	83
81	Self assembled fullerene walls in di-mesogenic-C60 materials. Soft Matter, 2009, 5, 4484.	1.2	13
82	A chirality index for investigating protein secondary structures and their time evolution. Proteins: Structure, Function and Bioinformatics, 2008, 70, 667-677.	1.5	37
83	Computer simulations of biaxial nematics. Journal of Physics Condensed Matter, 2008, 20, 463101.	0.7	106
84	Unveiling the Role of Histidine and Tyrosine Residues on the Conformation of the Avian Prion Hexarepeat Domain. Journal of Physical Chemistry B, 2008, 112, 5182-5188.	1.2	21
85	"Reduced" Distributed Monopole Model for the Efficient Prediction of Energy Transfer in Condensed Phases. Journal of Physical Chemistry B, 2008, 112, 1752-1760.	1.2	10
86	Field response and switching times in biaxial nematics. Journal of Chemical Physics, 2008, 128, 024905.	1.2	95
87	Charge Transport in Conjugated Materials: From Theoretical Models to Experimental Systems. AIP Conference Proceedings, 2008, , .	0.3	2
88	A computer simulation study of the formation of liquid crystal nanodroplets from a homogeneous solution. Journal of Chemical Physics, 2007, 126, 044905.	1.2	39
89	An NMR and molecular dynamics investigation of the avian prion hexarepeat conformational features in solution. Chemical Physics Letters, 2007, 442, 110-118.	1.2	12
90	Core charge distribution and self assembly of columnar phases: the case of triphenylenes and azatriphenylenes. Chemistry Central Journal, 2007, 1, 15.	2.6	20

#	Article	IF	Citations
91	Molecular properties and stacking of 1-substituted hexaalkoxy triphenylenes. Theoretical Chemistry Accounts, 2007, 117, 1085-1092.	0.5	10
92	A computer simulation of model discotic dimers. Theoretical Chemistry Accounts, 2007, 118, 203-210.	0.5	12
93	A deformable Gayâ€“Berne model for the simulation of liquid crystals and soft materials. Chemical Physics Letters, 2006, 423, 1-6.	1.2	12
94	Effect of nanoconfinement on liquid-crystal polymer chains. Journal of Chemical Physics, 2005, 123, 224705.	1.2	26
95	Can the Ï€-Facial Selectivity of Solvation Be Predicted by Atomistic Simulation?. Journal of the American Chemical Society, 2005, 127, 10699-10706.	6.6	27
96	A computer simulation study of the influence of a liquid crystal medium on polymerization. Journal of Chemical Physics, 2004, 121, 9123-9130.	1.2	24
97	Can Nematic Transitions Be Predicted By Atomistic Simulations? A Computational Study of The Oddâ€“Even Effect. ChemPhysChem, 2004, 5, 104-111.	1.0	114
98	Mimicking electrostatic interactions with a set of effective charges: a genetic algorithm. Chemical Physics Letters, 2004, 389, 373-378.	1.2	19
99	Is the alignment of nematics on a polymer slab always along the rubbing direction? A molecular dynamics study. Liquid Crystals, 0, , 1-11.	0.9	6