# Luca Muccioli

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | Highly emissive excitons with reduced exchange energy in thermally activated delayed fluorescent molecules. Nature Communications, 2019, 10, 597. | 5.8 | 253 |
| 2 | 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 |
| 3 | Ferroelectric Response and Induced Biaxiality in the Nematic Phase of Bentâ€Core Mesogens. Advanced Functional Materials, 2009, 19, 2592-2600. | 7.8 | 187 |
| 4 | 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 |
| 5 | 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 |
| 6 | How Does the Transâ€“Cis Photoisomerization of Azobenzene Take Place in Organic Solvents?. ChemPhysChem, 2010, 11, 1018-1028. | 1.0 | 140 |
| 7 | Electrostatic phenomena in organic semiconductors: fundamentals and implications for photovoltaics. Journal of Physics Condensed Matter, 2016, 28, 433002. | 0.7 | 131 |
| 8 | Energetics of Electronâ€“Hole Separation at P3HT/PCBM Heterojunctions. Journal of Physical Chemistry C, 2013, 117, 12981-12990. | 1.5 | 126 |
| 9 | Computational Design of Thermally Activated Delayed Fluorescence Materials: The Challenges Ahead. Journal of Physical Chemistry Letters, 2018, 9, 6149-6163. | 2.1 | 121 |
| 10 | Can Nematic Transitions Be Predicted By Atomistic Simulations? A Computational Study of The Oddâ€“Even Effect. ChemPhysChem, 2004, 5, 104-111. | 1.0 | 114 |
| 11 | 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 |
| 12 | Computer simulations of biaxial nematics. Journal of Physics Condensed Matter, 2008, 20, 463101. | 0.7 | 106 |
| 13 | Nature of the singlet and triplet excitations mediating thermally activated delayed fluorescence. Physical Review Materials, 2017, 1, . | 0.9 | 102 |
| 14 | 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 |
| 15 | Field response and switching times in biaxial nematics. Journal of Chemical Physics, 2008, 128, 024905. | 1.2 | 95 |
| 16 | Charge Separation and Recombination at Polymerâ€“Fullerene Heterojunctions: Delocalization and Hybridization Effects. Journal of Physical Chemistry Letters, 2016, 7, 536-540. | 2.1 | 93 |
| 17 | Simulation of Vaporâ€Phase Deposition and Growth of a Pentacene Thin Film on C<sub>60</sub> (001). Advanced Materials, 2011, 23, 4532-4536. | 11.1 | 90 |
| 18 | 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 |

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|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | Assemblies of perylene diimide derivatives with melamine into luminescent hydrogels. Chemical Communications, 2011, 47, 11858. | 2.2 | 73 |
| 22 | 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 |
| 23 | Predicting surface anchoring: molecular organization across a thin film of 5CB liquid crystal on silicon. Chemical Science, 2012, 3, 573-579. | 3.7 | 69 |
| 24 | 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 |
| 25 | 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 |
| 26 | 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 |
| 27 | 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 |
| 28 | Orientation dependent molecular electrostatics drives efficient charge generation in homojunction organic solar cells. Nature Communications, 2020, 11, 4617. | 5.8 | 60 |
| 29 | An atomistic simulation of the liquid-crystalline phases of sexithiophene. Journal of Materials Chemistry, 2011, 21, 125-133. | 6.7 | 59 |
| 30 | 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 |
| 31 | 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 |
| 32 | Do charges delocalize over multiple molecules in fullerene derivatives?. Journal of Materials Chemistry C, 2016, 4, 3747-3756. | 2.7 | 44 |
| 33 | Structural Characterization of Alkylsilane and Fluoroalkylsilane Self-Assembled Monolayers on SiO<sub>2</sub> by Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 14652-14662. | 1.5 | 42 |
| 34 | 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 |
| 35 | Multi-dimensional charge transport in supramolecular helical foldamer assemblies. Chemical Science, 2017, 8, 7251-7257. | 3.7 | 38 |
| 36 | A chirality index for investigating protein secondary structures and their time evolution. Proteins: Structure, Function and Bioinformatics, 2008, 70, 667-677. | 1.5 | 37 |

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| 37 | 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 |
| 38 | Second-order nonlinear optical properties of Stenhouse photoswitches: insights from density functional theory. Physical Chemistry Chemical Physics, 2018, 20, 27658-27667. | 1.3 | 37 |
| 39 | Order and Conformation of Biphenyl in Cyanobiphenyl Liquid Crystals: A Combined Atomistic Molecular Dynamics and <sup>1</sup>H NMR Study. ChemPhysChem, 2014, 15, 1356-1367. | 1.0 | 33 |
| 40 | From Chiral Islands to Smectic Layers: A Computational Journey Across Sexithiophene Morphologies on C<sub>60</sub>. Advanced Functional Materials, 2015, 25, 1985-1995. | 7.8 | 32 |
| 41 | Quinquephenyl: The Simplest Rigidâ€Rodâ€Like Nematic Liquid Crystal, or is it? An Atomistic Simulation. ChemPhysChem, 2014, 15, 1345-1355. | 1.0 | 30 |
| 42 | 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 |
| 43 | Does supramolecular ordering influence exciton transport in conjugated systems? Insight from atomistic simulations. Chemical Science, 2011, 2, 1025. | 3.7 | 28 |
| 44 | Unusual electromechanical response in rubrene single crystals. Materials Horizons, 2018, 5, 41-50. | 6.4 | 28 |
| 45 | 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 |
| 46 | 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 |
| 47 | Effect of nanoconfinement on liquid-crystal polymer chains. Journal of Chemical Physics, 2005, 123, 224705. | 1.2 | 26 |
| 48 | 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 |
| 49 | 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 |
| 50 | Nonlinear Optical Contrast in Azobenzene-Based Self-Assembled Monolayers. Chemistry of Materials, 2019, 31, 6759-6769. | 3.2 | 25 |
| 51 | 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 |
| 52 | Dynamical Behavior and Second Harmonic Generation Responses in Acido-Triggered Molecular Switches. Journal of Physical Chemistry C, 2018, 122, 26160-26168. | 1.5 | 24 |
| 53 | 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 |
| 54 | 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 |

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| 55 | Energetic fluctuations in amorphous semiconducting polymers: Impact on charge-carrier mobility. Journal of Chemical Physics, 2017, 147, 134904. | 1.2 | 21 |
| 56 | 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 |
| 57 | Core charge distribution and self assembly of columnar phases: the case of triphenylenes and azatriphenylenes. Chemistry Central Journal, 2007, 1, 15. | 2.6 | 20 |
| 58 | 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 |
| 59 | Multiple Charge Transfer States in Donorâ€“Acceptor Heterojunctions with Large Frontier Orbital Energy Offsets. Chemistry of Materials, 2019, 31, 6808-6817. | 3.2 | 20 |
| 60 | Mimicking electrostatic interactions with a set of effective charges: a genetic algorithm. Chemical Physics Letters, 2004, 389, 373-378. | 1.2 | 19 |
| 61 | 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 |
| 62 | 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 |
| 63 | 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 |
| 64 | 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 |
| 65 | 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 |
| 66 | Temperature dependence of charge mobility in model discotic liquid crystals. Physical Chemistry Chemical Physics, 2012, 14, 5368. | 1.3 | 16 |
| 67 | Molecular organization in freely suspended nano-thick 8CB smectic films. An atomistic simulation. Physical Chemistry Chemical Physics, 2015, 17, 26149-26159. | 1.3 | 16 |
| 68 | 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 |
| 69 | Self-organization of complete organic monolayers via sequential post-deposition annealing. Progress in Organic Coatings, 2020, 138, 105408. | 1.9 | 15 |
| 70 | Nonlinear optical responses of self-assembled monolayers functionalized with indolinoâ€“oxazolidine photoswitches. Physical Chemistry Chemical Physics, 2018, 20, 21590-21597. | 1.3 | 14 |
| 71 | Self assembled fullerene walls in di-mesogenic-C60 materials. Soft Matter, 2009, 5, 4484. | 1.2 | 13 |
| 72 | Communication: Molecular dynamics and 1H NMR of n-hexane in liquid crystals. Journal of Chemical Physics, 2015, 143, 011103. | 1.2 | 13 |

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| 73 | A deformable Gayâ€“Berne model for the simulation of liquid crystals and soft materials. Chemical Physics Letters, 2006, 423, 1-6. | 1.2 | 12 |
| 74 | 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 |
| 75 | A computer simulation of model discotic dimers. Theoretical Chemistry Accounts, 2007, 118, 203-210. | 0.5 | 12 |
| 76 | Carbazole-based Ï€-conjugated polyazomethines: Effects of catenation and comonomer insertion on optoelectronic features. Polymer, 2017, 119, 274-284. | 1.8 | 12 |
| 77 | Molecular properties and stacking of 1-substituted hexaalkoxy triphenylenes. Theoretical Chemistry Accounts, 2007, 117, 1085-1092. | 0.5 | 10 |
| 78 | "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 |
| 79 | Application of Rubrene Air-Gap Transistors as Sensitive MEMS Physical Sensors. ACS Applied Materials & Interfaces, 2018, 10, 41570-41577. | 4.0 | 10 |
| 80 | Impact of structural anisotropy on electro-mechanical response in crystalline organic semiconductors. Journal of Materials Chemistry C, 2019, 7, 4382-4391. | 2.7 | 10 |
| 81 | 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 |
| 82 | Nâ€doped cycloparaphenylenes: Tuning electronic properties for applications in thermally activated delayed fluorescence. International Journal of Quantum Chemistry, 2018, 118, e25562. | 1.0 | 9 |
| 83 | 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 |
| 84 | Self-assembling, structure and nonlinear optical properties of fluorescent organic nanoparticles in water. Physical Chemistry Chemical Physics, 2021, 23, 23643-23654. | 1.3 | 9 |
| 85 | 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 |
| 86 | Surface-Confined Macrocyclization via Dynamic Covalent Chemistry. ACS Nano, 2020, 14, 2956-2965. | 7.3 | 8 |
| 87 | Structure and Charge Transport Properties of Cycloparaphenylene Monolayers on Graphite. Advanced Materials Interfaces, 2019, 6, 1801948. | 1.9 | 7 |
| 88 | Atomistic simulations of charge transport in photoswitchable organic-graphene hybrids. JPhys Materials, 2019, 2, 035001. | 1.8 | 7 |
| 89 | 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 |
| 90 | Peptoids as a Chiral Stationary Phase for Liquid Chromatography: Insights from Molecular Dynamics Simulations. Biomacromolecules, 2021, 22, 2573-2581. | 2.6 | 6 |

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| 91 | 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 |
| 92 | From rod-like to disc-like Gayâ€“Berne biaxial nematics and back. Liquid Crystals, 2018, 45, 2400-2415. | 0.9 | 4 |
| 93 | Bidimensional Hâ€Bond Network Promotes Structural Order and Electron Transport in BPyMPMs Molecular Semiconductor. Advanced Theory and Simulations, 2021, 4, 2000302. | 1.3 | 4 |
| 94 | 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 |
| 95 | 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 |
| 96 | Charge Transport in Conjugated Materials: From Theoretical Models to Experimental Systems. AIP Conference Proceedings, 2008, , . | 0.3 | 2 |
| 97 | Pressure sensor based on organic single crystal air-gap transistor. , 2017, , . | | 1 |
| 98 | A Festschrift in honour of Professor Claudio Zannoni. Liquid Crystals, 2018, 45, 1871-1879. | 0.9 | 0 |
| 99 | Direct Triple Annulations: A Way to Design Large Triazastarphenes with Intertwined Hexagonal Packing. Organic Letters, 2022, 24, 344-348. | 2.4 | 0 |