

Antonino Famulari

List of Publications by Year in descending order

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68
papers

1,927
citations

236925

25
h-index

276875

41
g-index

70
all docs

70
docs citations

70
times ranked

2388
citing authors

#	ARTICLE	IF	CITATIONS
1	Dual-Mode Light Transduction through a Plastically Bendable Organic Crystal as an Optical Waveguide. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 17254-17258.	13.8	169
2	Computational reinvestigation of the bithiophene torsion potential. <i>Chemical Physics Letters</i> , 2003, 379, 364-372.	2.6	121
3	Structural Organization and Transport Properties of Novel Pyrrolidinium-Based Ionic Liquids with Perfluoroalkyl Sulfonylimide Anions. <i>Journal of Physical Chemistry B</i> , 2009, 113, 10750-10759.	2.6	102
4	Blending ionic liquids: how physico-chemical properties change. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1784.	2.8	69
5	Pyrrolidinium-Based Ionic Liquids Doped with Lithium Salts: How Does Li ⁺ Coordination Affect Its Diffusivity?. <i>Journal of Physical Chemistry B</i> , 2014, 118, 13679-13688.	2.6	63
6	2,9-Dicarbonyl-1,10-phenanthroline derivatives with an unprecedented Am(III)/Eu(III) selectivity under highly acidic conditions. <i>Dalton Transactions</i> , 2013, 42, 16930.	3.3	58
7	Synthesis and characterization of new electron acceptor perylene diimide molecules for photovoltaic applications. <i>Dyes and Pigments</i> , 2013, 99, 329-338.	3.7	56
8	Structure and morphology of HDPE-g-MA/organoclay nanocomposites: Effects of the preparation procedures. <i>European Polymer Journal</i> , 2008, 44, 987-1002.	5.4	54
9	Ordered Stacking of Regioregular Head-to-Tail Polyalkylthiophenes: Insights from the Crystal Structure of Form I ² Poly(3-hexylthiophene). <i>Chemistry of Materials</i> , 2009, 21, 78-87.	6.7	50
10	Pyrazolium- versus Imidazolium-Based Ionic Liquids: Structure, Dynamics and Physicochemical Properties. <i>Journal of Physical Chemistry B</i> , 2013, 117, 668-676.	2.6	49
11	Direct trifluoro-methoxylation of aromatics with perfluoro-methyl-hypofluorite. <i>Journal of Fluorine Chemistry</i> , 2012, 140, 43-48.	1.7	48
12	Interplay of Conformational States and Nonbonded Interactions in Substituted Bithiophenes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 691-698.	2.5	44
13	Preparation and characterization of superhydrophobic conductive fluorinated carbon blacks. <i>Carbon</i> , 2010, 48, 4382-4390.	10.3	43
14	Functionalization of multi-walled carbon nanotubes with perfluoropolyether peroxide to produce superhydrophobic properties. <i>Carbon</i> , 2013, 59, 150-159.	10.3	43
15	Dualmodus-Lichttransduktion durch einen plastisch biegbaren organischen Kristall als optischer Wellenleiter. <i>Angewandte Chemie</i> , 2018, 130, 17501-17505.	2.0	41
16	Solid-State Optical and Structural Modifications Induced by Temperature in a Chiral Poly-3-alkylthiophene. <i>Chemistry of Materials</i> , 2002, 14, 4819-4826.	6.7	38
17	Synthesis, Characterization, and Crystalline Structure of Syndiotactic 1,2-Polypentadiene: The Trans Polymer. <i>Macromolecules</i> , 2005, 38, 8345-8352.	4.8	38
18	Structure-Photoluminescence Correlation for Two Crystalline Polymorphs of a Thiophene-Phenylene Co-Oligomer with Bulky Terminal Substituents. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2171-2176.	4.6	37

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19	Analysis of the Reactivity on the C ₇ H ₆ Potential Energy Surface. Journal of Physical Chemistry A, 2011, 115, 7928-7936.	2.5	32
20	Intramolecular CH/π interactions in alkylaromatics: Monomer conformations for poly(3-alkylthiophene) atomistic models. International Journal of Quantum Chemistry, 2013, 113, 2154-2162.	2.0	31
21	Mechanochemical dehydrochlorination and chelation reaction in the solid state: from a molecular salt to a coordination complex. CrystEngComm, 2014, 16, 969-973.	2.6	31
22	Solid state transformations in stoichiometric hydrogen bonded molecular salts: ionic interconversion and dehydration processes. CrystEngComm, 2013, 15, 6237.	2.6	30
23	Synthesis of Chelating Complexes through Solid-State Dehydrochlorination Reactions via Second-Sphere-Coordination Interaction with Metal Chlorides: A Combined Experimental/Molecular Modeling Study. Inorganic Chemistry, 2014, 53, 7438-7445.	4.0	30
24	<i>N</i> -Alkyl substituted 1 <i>H</i> -benzimidazoles as improved n-type dopants for a naphthalene-diimide based copolymer. Journal of Materials Chemistry A, 2018, 6, 15294-15302.	10.3	28
25	First Detailed Determination of the Molecular Conformation and the Crystalline Packing of a Chiral Poly(3-alkylthiophene): Poly-3-(S)-2-methylbutylthiophene. Macromolecules, 2007, 40, 3-5.	4.8	27
26	A Solid State Density Functional Study of Crystalline Thiophene-Based Oligomers and Polymers. Journal of Physical Chemistry B, 2012, 116, 14504-14509.	2.6	27
27	Gas/Solid Chemisorption/Adsorption and Mechanochemical Selectivity in Dynamic Nonporous Hybrid Metal Organic Materials. Inorganic Chemistry, 2017, 56, 6584-6590.	4.0	27
28	On the inter-ring torsion potential of regioregular P3HT: a first principles reexamination with explicit side chains. Physical Chemistry Chemical Physics, 2014, 16, 3983.	2.8	26
29	Chain statistics in polyethylene crystallization. Polymer, 2009, 50, 1819-1829.	3.8	25
30	A Combined Experimental and Theoretical Study on the Stereodynamics of Monoaza[5]helicenes: Solvent-Induced Increase of the Enantiomerization Barrier in 1-aza[5]helicene. Chemistry - A European Journal, 2015, 21, 13919-13924.	3.3	25
31	4,4'-Dipyridyl Dioxide-SbF ₃ Cocrystal: Pnictogen Bond Prevails over Halogen and Hydrogen Bonds in Driving Self-Assembly. Crystal Growth and Design, 2020, 20, 916-922.	3.0	25
32	Tuning the Inclusion Properties and Solid-State Reactivity of Second Sphere Adducts Using Conformationally Flexible Bidentate Ligands. Crystal Growth and Design, 2015, 15, 2842-2852.	3.0	24
33	An orthogonal approach to determine extremely localised molecular orbitals. Theoretical Chemistry Accounts, 2000, 103, 417-422.	1.4	22
34	Improving the efficiency of P3HT:perylene diimide solar cells via bay-substitution with fused aromatic rings. RSC Advances, 2013, 3, 9185.	3.6	22
35	Kinetically Controlled Fast Crystallization of M ₁₂ L ₈ Poly-[<i>n</i>]-catenanes Using the 2,4,6-Tris(4-pyridyl)benzene Ligand and ZnCl ₂ in an Aromatic Environment. Journal of the American Chemical Society, 2020, 142, 9537-9543.	13.7	22
36	Titanium-Catalyzed Norbornene Oligomerization. Isolation of a Crystalline Heptamer with a 2,3-exo-Disyndiotactic Structure. Macromolecular Rapid Communications, 2006, 27, 1937-1941.	3.9	21

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37	Synthesis and structural characterization of syndiotactic <i>trans</i> -1,2 and <i>cis</i> -1,2 polyhexadienes. <i>Journal of Polymer Science Part A</i> , 2007, 45, 5339-5353.	2.3	21
38	Peroxidic perfluoropolyether for the covalent binding of perfluoropolyether chains on carbon black surface. <i>Journal of Fluorine Chemistry</i> , 2011, 132, 1254-1261.	1.7	21
39	Synthesis, Characterization and Molecular Conformation of Syndiotactic 1,2 Polypentadiene: The Cis Polymer. <i>Macromolecules</i> , 2005, 38, 8353-8361.	4.8	19
40	Oxoanion Binding by Guanidiniocarbonylpyrrole Cations in Water: A Combined DFT and MD Investigation. <i>Chemistry - A European Journal</i> , 2008, 14, 5207-5219.	3.3	18
41	Structural and energetic aspects of a new bupropion hydrochloride polymorph. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2012, 60, 65-70.	2.8	18
42	New Stereoregularity in the Stereospecific Polymerization of Bulky Strained Olefins: Diheterotactic Polynorbornene. <i>Macromolecules</i> , 2008, 41, 3109-3113.	4.8	16
43	Exploiting polymorphism in second sphere coordination: thermal transformation, NLO properties and selective mechanochemical synthesis. <i>CrystEngComm</i> , 2016, 18, 2408-2412.	2.6	16
44	Insights into the electron-donating and withdrawing effect of the functional groups on mechanochemical dehydrochlorination reactions. <i>Dalton Transactions</i> , 2017, 46, 9466-9471.	3.3	16
45	Insights into the formation of chiral second sphere coordination complexes with aromatic tris amines: combined single crystal X-ray crystallography and molecular modeling analyses. <i>Dalton Transactions</i> , 2015, 44, 15960-15965.	3.3	14
46	2,3- <i>exo</i> -Disyndiotactic Polynorbornene: A Crystalline Polymer with Tubular Helical Molecular Structure. <i>Macromolecules</i> , 2011, 44, 3681-3684.	4.8	13
47	Quantum Mechanics Calculations, Basicity and Crystal Structure: The Route to Transition Metal Complexes of Azahelicenes. <i>Molecules</i> , 2012, 17, 463-479.	3.8	13
48	Chalcogen Bonds in Selenocysteine Seleninic Acid, a Functional GPx Constituent, and in Other Seleninic or Sulfinic Acid Derivatives. <i>Chemistry - an Asian Journal</i> , 2021, 16, 2351-2360.	3.3	12
49	Cyclic Interconversion among Molecular Salts via Neat Grinding and Related Photoluminescence Properties. <i>Crystal Growth and Design</i> , 2014, 14, 6528-6536.	3.0	11
50	Exploring short intramolecular interactions in alkylaromatic substrates. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29616-29628.	2.8	11
51	Dynamic behaviour in nonporous hybrid metal-organic materials via mechanochemical and gas-solid reactions. <i>CrystEngComm</i> , 2018, 20, 6721-6726.	2.6	10
52	Polymorphs and Transformations of the Solid Forms of Organic Salts of 5-Sulfosalicylic Acid and Isonicotinamide. <i>Crystal Growth and Design</i> , 2020, 20, 7606-7614.	3.0	10
53	Materials for organic photovoltaics: insights from detailed structural models and molecular simulations. <i>EPJ Web of Conferences</i> , 2012, 33, 02002.	0.3	9
54	Free-radical selective functionalization of 1,4-naphthoquinones by perfluorodiacyl peroxides. <i>Tetrahedron</i> , 2014, 70, 5298-5309.	1.9	9

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55	Mononuclear Ru(II) PolyPyridyl Water Oxidation Catalysts Decorated with Perfluoroalkyl C8 H17 -Tag Bearing Chains. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 4463-4470.	2.0	9
56	Environmentally Friendly and Regioselective One-Pot Synthesis of Imines and Oxazolidines Serinol Derivatives and Their Use for Rubber Cross-Linking. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 9356-9366.	6.7	9
57	Atomistic modelling of entropy driven phase transitions between different crystal modifications in polymers: the case of poly(3-alkylthiophenes). <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 28984-28989.	2.8	8
58	Combined structural and theoretical investigation on differently substituted bispidine ligands: predicting the properties of their corresponding coordination polymers. <i>Dalton Transactions</i> , 2020, 49, 5965-5973.	3.3	8
59	Structure and Electrical Bistability of a New Class of Diphenyl-bithiophenes: A Combined Theoretical and Experimental Study. <i>Journal of Physical Chemistry C</i> , 2008, 112, 18628-18637.	3.1	7
60	Reactivity among first and second coordination spheres using a multiprotonated ligand and Cu($\text{Cu}(\text{scpp})$) in the solid-state. <i>CrystEngComm</i> , 2019, 21, 4354-4362.	2.6	6
61	Host-Guest Chemistry of M_{12}L_8 Poly-[n]-catenanes: Inclusion Process by Switchable "Closed" "Open" Dynamic Channels. <i>Crystal Growth and Design</i> , 2022, 22, 4494-4502.	3.0	6
62	Experimental X-ray and DFT Structural Analyses of M_{12}L_8 Poly-[n]-catenanes Using exo-Tridentate Ligands. <i>Inorganic Chemistry</i> , 2022, 61, 10863-10871.	4.0	6
63	Stoichiometry mechanosynthesis and interconversion of metal salts containing $[\text{CuCl}_3(\text{H}_2\text{O})]^{2-}$ and $[\text{Cu}_2\text{Cl}_8]^{4-}$. <i>CrystEngComm</i> , 2019, 21, 7017-7024.	2.6	4
64	Nucleophilicity and electrophilicity of the $\text{C}(\text{sp}^3)\text{-H}$ bond: methane and ethane binary complexes with iodine. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 24555-24565.	2.8	3
65	Modeling of Poly(3-hexylthiophene) and Its Oligomer's Structure and Thermal Behavior with Different Force Fields: Insights into the Phase Transitions of Semiconducting Polymers. <i>Macromolecules</i> , 0, , .	4.8	3
66	Structural properties of the chelating agent 2,6-bis(1-(3-hydroxypropyl)-1,2,3-triazol-4-yl)pyridine: a combined XRD and DFT structural study. <i>RSC Advances</i> , 2020, 10, 19629-19635.	3.6	2
67	A haptic framework for the study of inter-molecular interactions. <i>International Journal of Technology Enhanced Learning</i> , 2011, 3, 536.	0.7	1
68	Synthesis and structural properties of isostructural $\text{Zn}_{12}\text{M}_{12}\text{L}_8$ poly-[n]-catenane using the 2,4,6-tris(4-pyridyl)benzene (TPB) ligand. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2021, 77, C166-C166.	0.1	0