Antonino Famulari

List of Publications by Year
in descending order

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	Hostâ€“Guest Chemistry of M₁₂L₈ Poly-[n]-catenanes: Inclusion Process by Switchable â€œClosedâ€“Openâ€•Dynamic Channels. Crystal Growth and Design, 2022, 22, 4494-4502.	3.0	6
2	Experimental X-ray and DFT Structural Analyses of M₁₂L₈ Poly-[n]-catenanes Using exo-Tridentate Ligands. Inorganic Chemistry, 2022, 61, 10863-10871.	4.0	6
3	Chalcogen Bonds in Selenocysteine Seleninic Acid, a Functional GPx Constituent, and in Other Seleninic or Sulfinic Acid Derivatives. Chemistry - an Asian Journal, 2021, 16, 2351-2360.	3.3	12
4	Synthesis and structural properties of isostructural Zn^{II} M ₁₂ L ₈ poly-[n]-catenane using the 2,4,6-tris(4-pyridyl)benzene (TPB) ligand. Acta Crystallographica Section A: Foundations and Advances, 2021, 77, C166-C166.	0.1	0
5	4,4â€²-Dipyridyl DioxideÂ·SbF₃ Cocrystal: Pnictogen Bond Prevails over Halogen and Hydrogen Bonds in Driving Self-Assembly. Crystal Growth and Design, 2020, 20, 916-922.	3.0	25
6	Polymorphs and Transformations of the Solid Forms of Organic Salts of 5-Sulfosalicylic Acid and Isonicotinamide. Crystal Growth and Design, 2020, 20, 7606-7614.	3.0	10
7	Environmentally Friendly and Regioselective One-Pot Synthesis of Imines and Oxazolidines Serinol Derivatives and Their Use for Rubber Cross-Linking. ACS Sustainable Chemistry and Engineering, 2020, 8, 9356-9366.	6.7	9
8	Kinetically Controlled Fast Crystallization of M₁₂L₈ Poly-[n]-catenanes Using the 2,4,6-Tris(4-pyridyl)benzene Ligand and ZnCl₂ in an Aromatic Environment. Journal of the American Chemical Society, 2020, 142, 9537-9543.	13.7	22
9	Combined structural and theoretical investigation on differently substituted bispidine ligands: predicting the properties of their corresponding coordination polymers. Dalton Transactions, 2020, 49, 5965-5973.	3.3	8
10	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. RSC Advances, 2020, 10, 19629-19635.	3.6	2
11	Mononuclear Ru(II) PolyPyridyl Water Oxidation Catalysts Decorated with Perfluoroalkyl C8 H17 -Tag Bearing Chains. European Journal of Inorganic Chemistry, 2019, 2019, 4463-4470.	2.0	9
12	Reactivity among first and second coordination spheres using a multiprotonated ligand and Cu(<scp>ii</scp>) in the solid-state. CrystEngComm, 2019, 21, 4354-4362.	2.6	6
13	Stoichiometry mechanosynthesis and interconversion of metal salts containing [CuCl₃(H₂O)]^{â^’} and [Cu₂Cl₈]^{4â^’}. CrystEngComm, 2019, 21, 7017-7024.	2.6	4
14	Atomistic modelling of entropy driven phase transitions between different crystal modifications in polymers: the case of poly(3-alkylthiophenes). Physical Chemistry Chemical Physics, 2018, 20, 28984-28989.	2.8	8
15	Dynamic behaviour in nonporous hybrid metalâ€“organic materials via mechanochemical and gasâ€“solid reactions. CrystEngComm, 2018, 20, 6721-6726.	2.6	10
16	Dualmodusâ€Lichttransduktion durch einen plastisch biegbaren organischen Kristall als optischer Wellenleiter. Angewandte Chemie, 2018, 130, 17501-17505.	2.0	41
17	Dualâ€Mode Light Transduction through a Plastically Bendable Organic Crystal as an Optical Waveguide. Angewandte Chemie - International Edition, 2018, 57, 17254-17258.	13.8	169
18	N-Alkyl substituted 1H-benzimidazoles as improved n-type dopants for a naphthalene-diimide based copolymer. Journal of Materials Chemistry A, 2018, 6, 15294-15302.	10.3	28

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19	Gasâ€“Solid Chemisorption/Adsorption and Mechanochemical Selectivity in Dynamic Nonporous Hybrid Metal Organic Materials. Inorganic Chemistry, 2017, 56, 6584-6590.	4.0	27
20	Nucleophilicity and electrophilicity of the C(sp³)â€“H bond: methane and ethane binary complexes with iodine. Physical Chemistry Chemical Physics, 2017, 19, 24555-24565.	2.8	3
21	Insights into the electron-donating and withdrawing effect of the functional groups on mechanochemical dehydrochlorination reactions. Dalton Transactions, 2017, 46, 9466-9471.	3.3	16
22	Exploring short intramolecular interactions in alkylaromatic substrates. Physical Chemistry Chemical Physics, 2016, 18, 29616-29628.	2.8	11
23	Exploiting polymorphism in second sphere coordination: thermal transformation, NLO properties and selective mechanochemical synthesis. CrystEngComm, 2016, 18, 2408-2412.	2.6	16
24	Insights into the formation of chiral second sphere coordination complexes with aromatic tris amines: combined single crystal X-ray crystallography and molecular modeling analyses. Dalton Transactions, 2015, 44, 15960-15965.	3.3	14
25	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
26	A Combined Experimental and Theoretical Study on the Stereodynamics of Monoaza[5]helicenes: Solventâ€Induced Increase of the Enantiomerization Barrier in 1â€Azaâ€[5]helicene. Chemistry - A European Journal, 2015, 21, 13919-13924.	3.3	25
27	Pyrrolidinium-Based Ionic Liquids Doped with Lithium Salts: How Does Li⁺ Coordination Affect Its Diffusivity?. Journal of Physical Chemistry B, 2014, 118, 13679-13688.	2.6	63
28	Cyclic Interconversion among Molecular Salts via Neat Grinding and Related Photoluminescence Properties. Crystal Growth and Design, 2014, 14, 6528-6536.	3.0	11
29	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
30	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
31	Structureâ€“Photoluminescence Correlation for Two Crystalline Polymorphs of a Thiopheneâ€“Phenylene Co-Oligomer with Bulky Terminal Substituents. Journal of Physical Chemistry Letters, 2014, 5, 2171-2176.	4.6	37
32	Synthesis of Chelating Complexes through Solid-State Dehydrochlorination Reactions via Second-Sphere-Coordination Interaction with Metal Chlorides: A Combined Experimentalâ€“Molecular Modeling Study. Inorganic Chemistry, 2014, 53, 7438-7445.	4.0	30
33	Free-radical selective functionalization of 1,4-naphthoquinones by perfluorodiacyl peroxides. Tetrahedron, 2014, 70, 5298-5309.	1.9	9
34	Solid state transformations in stoichiometric hydrogen bonded molecular salts: ionic interconversion and dehydration processes. CrystEngComm, 2013, 15, 6237.	2.6	30
35	2,9-Dicarbonyl-1,10-phenanthroline derivatives with an unprecedented Am(iii)/Eu(iii) selectivity under highly acidic conditions. Dalton Transactions, 2013, 42, 16930.	3.3	58
36	Intramolecular CH/Ï€ interactions in alkylaromatics: Monomer conformations for poly(3â€alkylthiophene) atomistic models. International Journal of Quantum Chemistry, 2013, 113, 2154-2162.	2.0	31

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37	Pyrazolium- versus Imidazolium-Based Ionic Liquids: Structure, Dynamics and Physicochemical Properties. Journal of Physical Chemistry B, 2013, 117, 668-676.	2.6	49
38	Improving the efficiency of P3HT:perylene diimide solar cells via bay-substitution with fused aromatic rings. RSC Advances, 2013, 3, 9185.	3.6	22
39	Synthesis and characterization of new electron acceptor perylene diimide molecules for photovoltaic applications. Dyes and Pigments, 2013, 99, 329-338.	3.7	56
40	Functionalization of multi-walled carbon nanotubes with perfluoropolyether peroxide to produce superhydrophobic properties. Carbon, 2013, 59, 150-159.	10.3	43
41	Materials for organic photovoltaics: insights from detailed structural models and molecular simulations. EPJ Web of Conferences, 2012, 33, 02002.	0.3	9
42	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
43	Quantum Mechanics Calculations, Basicity and Crystal Structure: The Route to Transition Metal Complexes of Azahelicenes. Molecules, 2012, 17, 463-479.	3.8	13
44	Structural and energetic aspects of a new bupropion hydrochloride polymorph. Journal of Pharmaceutical and Biomedical Analysis, 2012, 60, 65-70.	2.8	18
45	Direct trifluoro-methoxylation of aromatics with perfluoro-methyl-hypofluorite. Journal of Fluorine Chemistry, 2012, 140, 43-48.	1.7	48
46	2,3-exo-Disyndiotactic Polynorbornene: A Crystalline Polymer with Tubular Helical Molecular Structure. Macromolecules, 2011, 44, 3681-3684.	4.8	13
47	Analysis of the Reactivity on the C₇H₆ Potential Energy Surface. Journal of Physical Chemistry A, 2011, 115, 7928-7936.	2.5	32
48	A haptic framework for the study of inter-molecular interactions. International Journal of Technology Enhanced Learning, 2011, 3, 536.	0.7	1
49	Peroxidic perfluoropolyether for the covalent binding of perfluoropolyether chains on carbon black surface. Journal of Fluorine Chemistry, 2011, 132, 1254-1261.	1.7	21
50	Preparation and characterization of superhydrophobic conductive fluorinated carbon blacks. Carbon, 2010, 48, 4382-4390.	10.3	43
51	Blending ionic liquids: how physico-chemical properties change. Physical Chemistry Chemical Physics, 2010, 12, 1784.	2.8	69
52	Chain statistics in polyethylene crystallization. Polymer, 2009, 50, 1819-1829.	3.8	25
53	Ordered Stacking of Regioregular Head-to-Tail Polyalkylthiophenes: Insights from the Crystal Structure of Form Iâ€² Poly(3-n-butylthiophene). Chemistry of Materials, 2009, 21, 78-87.	6.7	50
54	Structural Organization and Transport Properties of Novel Pyrrolidinium-Based Ionic Liquids with Perfluoroalkyl Sulfonylimide Anions. Journal of Physical Chemistry B, 2009, 113, 10750-10759.	2.6	102

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55	Oxoanion Binding by Guanidiniocarbonylpyrrole Cations in Water: A Combined DFT and MD Investigation. Chemistry - A European Journal, 2008, 14, 5207-5219.	3.3	18
56	Structure and morphology of HDPE-g-MA/organoclay nanocomposites: Effects of the preparation procedures. European Polymer Journal, 2008, 44, 987-1002.	5.4	54
57	Structure and Electrical Bistability of a New Class of Diphenyl-bithiophenes: A Combined Theoretical and Experimental Study. Journal of Physical Chemistry C, 2008, 112, 18628-18637.	3.1	7
58	New Stereoregularity in the Stereospecific Polymerization of Bulky Strained Olefins: Diheterotactic Polynorbornene. Macromolecules, 2008, 41, 3109-3113.	4.8	16
59	First Detailed Determination of the Molecular Conformation and the Crystalline Packing of a Chiral Poly(3-alkylthiophene):Â Poly-3-(S)-2-methylbutylthiophene. Macromolecules, 2007, 40, 3-5.	4.8	27
60	Synthesis and structural characterization of syndiotactic transâ€1,2 and cisâ€1,2 polyhexadienes. Journal of Polymer Science Part A, 2007, 45, 5339-5353.	2.3	21
61	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
62	Synthesis, Characterization and Molecular Conformation of Syndiotactic 1,2 Polypentadiene:Â The Cis Polymer. Macromolecules, 2005, 38, 8353-8361.	4.8	19
63	Synthesis, Characterization, and Crystalline Structure of Syndiotactic 1,2-Polypentadiene:Â The Trans Polymer. Macromolecules, 2005, 38, 8345-8352.	4.8	38
64	Interplay of Conformational States and Nonbonded Interactions in Substituted Bithiophenes. Journal of Physical Chemistry A, 2004, 108, 691-698.	2.5	44
65	Computational reinvestigation of the bithiophene torsion potential. Chemical Physics Letters, 2003, 379, 364-372.	2.6	121
66	Solid-State Optical and Structural Modifications Induced by Temperature in a Chiral Poly-3-alkylthiophene. Chemistry of Materials, 2002, 14, 4819-4826.	6.7	38
67	An orthogonal approach to determine extremely localised molecular orbitals. Theoretical Chemistry Accounts, 2000, 103, 417-422.	1.4	22
68	Modeling of Poly(3-hexylthiophene) and Its Oligomerâ€™s Structure and Thermal Behavior with Different Force Fields: Insights into the Phase Transitions of Semiconducting Polymers. Macromolecules, 0, , .	4.8	3