Juan AragÃ³

List of Publications by Year
in descending order

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82	2,148	201385 27	253896 43
papers	citations	h-index	g-index

85	85	85	3276
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Influence of the Z/E Isomerism on the Pathway Complexity of a Squaramideâ€Based Macrocycle. Small, 2021, 17, e2006133.	5.2	14
2	Effect of molecular geometry and extended conjugation on the performance of hydrogen-bonded semiconductors in organic thin-film field-effect transistors. Journal of Materials Chemistry C, 2021, 9, 10819-10829.	2.7	5
3	Improving the Robustness of Organic Semiconductors through Hydrogen Bonding. ACS Applied Materials & Interfaces, 2021, 13, 8620-8630.	4.0	13
4	Effect of Substituents at Imide Positions on the Laser Performance of 1,7-Bay-Substituted Perylenediimide Dyes. Journal of Physical Chemistry C, 2021, 125, 12277-12288.	1.5	7
5	Hole-Transporting Materials for Perovskite Solar Cells Employing an Anthradithiophene Core. ACS Applied Materials & Interfaces, 2021, 13, 28214-28221.	4.0	30
6	Self-Assembly-Directed Organization of a Fullereneâ€“Bisporphyrin into Supramolecular Giant Donut Structures for Excited-State Charge Stabilization. Journal of the American Chemical Society, 2021, 143, 11199-11208.	6.6	6
7	Selenopheneâ€Based Holeâ€Transporting Materials for Perovskite Solar Cells. ChemPlusChem, 2021, 86, 1006-1013.	1.3	7
8	Binding Sites, Vibrations and Spinâ€Lattice Relaxation Times in Europium(II)â€Based Metallofullerene Spin Qubits. Chemistry - A European Journal, 2021, 27, 13242-13248.	1.7	7
9	Spectroscopic Analysis of Vibronic Relaxation Pathways in Molecular Spin Qubit [Ho(W₅O₁₈)₂]^{9â€“}: Sparse Spectra Are Key. Inorganic Chemistry, 2021, 60, 14096-14104.	1.9	22
10	Distance Matters: Biasing Mechanism, Transfer of Asymmetry, and Stereomutation in N-Annulated Perylene Bisimide Supramolecular Polymers. Journal of the American Chemical Society, 2021, 143, 13281-13291.	6.6	43
11	Supramolecular assembly of pyrene-tetrathiafulvalene hybrids on graphene: structureâ€“property relationships and biosensing activity. Journal of Materials Chemistry C, 2021, 9, 10944-10951.	2.7	6
12	Enhanced electronic communication through a conjugated bridge in a porphyrinâ€“fullerene donorâ€“acceptor couple. Journal of Materials Chemistry C, 2021, 9, 10889-10898.	2.7	3
13	Improving the Longâ€Term Stability of Doped Spiroâ€Type Holeâ€Transporting Materials in Planar Perovskite Solar Cells. Solar Rrl, 2021, 5, 2100650.	3.1	6
14	Charge-Separation and Charge-Recombination Rate Constants in a Donorâ€“Acceptor Buckybowl-Based Supramolecular Complex: Multistate and Solvent Effects. Journal of Physical Chemistry A, 2021, 125, 9982-9994.	1.1	3
15	Ternary Organic Solar Cell with a Nearâ€Infrared Absorbing Selenopheneâ€“Diketopyrrolopyrroleâ€Based Nonfullerene Acceptor and an Efficiency above 10%. Solar Rrl, 2020, 4, 1900471.	3.1	21
16	Tetrasubstituted Thieno[3,2-b]thiophenes as Hole-Transporting Materials for Perovskite Solar Cells. Journal of Organic Chemistry, 2020, 85, 224-233.	1.7	20
17	Dual-Mode Chiral Self-Assembly of Cone-Shaped Subphthalocyanine Aromatics. Journal of the American Chemical Society, 2020, 142, 21017-21031.	6.6	32
18	Impact of Molecular Size and Shape on the Supramolecular Coâ€Assembly of Chiral Tricarboxamides: A Comparative Study. Chemistry - A European Journal, 2020, 26, 14700-14707.	1.7	9

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19	Azatruxeneâ€Based, Dumbbellâ€Shaped, Donorâ€“Ïâ€Bridgeâ€“Donor Holeâ€Transporting Materials for Perovskite Solar Cells. Chemistry - A European Journal, 2020, 26, 11039-11047.	1.7	15
20	On the Structure and Chiral Aggregation of Liquid Crystalline Starâ€Shaped Triazines Hâ€Bonded to Benzoic Acids. Chemistry - A European Journal, 2020, 26, 15313-15322.	1.7	5
21	Flipping Motion To Bias the Organized Supramolecular Polymerization of N-Heterotriangulenes. Chemistry of Materials, 2019, 31, 7024-7032.	3.2	10
22	Understanding the affinity of bis-exTTF macrocyclic receptors towards fullerene recognition. Physical Chemistry Chemical Physics, 2019, 21, 11670-11675.	1.3	12
23	Saddle-like, Ï€-conjugated, cyclooctatetrathiophene-based, hole-transporting material for perovskite solar cells. Journal of Materials Chemistry C, 2019, 7, 6656-6663.	2.7	27
24	Nonâ€Planar and Flexible Holeâ€Transporting Materials from Bisâ€Xanthene and Bisâ€Thioxanthene Units for Perovskite Solar Cells. Helvetica Chimica Acta, 2019, 102, e1900056.	1.0	3
25	Decoding the Consequences of Increasing the Size of Self-Assembling Tricarboxamides on Chiral Amplification. Journal of the American Chemical Society, 2019, 141, 7463-7472.	6.6	44
26	Minimizing geminate recombination losses in small-molecule-based organic solar cells. Journal of Materials Chemistry C, 2019, 7, 6641-6648.	2.7	5
27	In Silico Molecular Engineering of Dysprosocenium-Based Complexes to Decouple Spin Energy Levels from Molecular Vibrations. Journal of Physical Chemistry Letters, 2019, 10, 7678-7683.	2.1	39
28	Selfâ€Assembly of Clicked Starâ€Shaped Triazines into Functional Nanostructures. ChemNanoMat, 2019, 5, 130-137.	1.5	2
29	Dibenzoquinquethiophene- and Dibenzosexithiophene-Based Hole-Transporting Materials for Perovskite Solar Cells. Chemistry of Materials, 2019, 31, 6435-6442.	3.2	46
30	Hole transporting materials based on benzodithiophene and dithienopyrrole cores for efficient perovskite solar cells. Journal of Materials Chemistry A, 2018, 6, 5944-5951.	5.2	44
31	Frontispiece: Hierarchy of Asymmetry at Work: Chainâ€Dependent Helixâ€toâ€Helix Interactions in Supramolecular Polymers. Chemistry - A European Journal, 2018, 24, .	1.7	0
32	Hierarchy of Asymmetry at Work: Chainâ€Dependent Helixâ€toâ€Helix Interactions in Supramolecular Polymers. Chemistry - A European Journal, 2018, 24, 2826-2831.	1.7	25
33	Tuning the optical and electronic properties of perylene diimides through transversal core extension. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	3
34	Bending Carbon Nanoforms for Supramolecular Recognition: A Topological Study on Hemifullerene-Based Aggregates. Journal of Physical Chemistry A, 2018, 122, 1124-1137.	1.1	5
35	Tuning the electronic properties and the planarity degree in the Ï€-extended TTF series: the prominent role of heteroatoms. Journal of Materials Chemistry C, 2018, 6, 13190-13196.	2.7	4
36	Synergy of Axial and Point Chirality to Construct Helical Nâ€Heterotriangleneâ€Based Supramolecular Polymers. ChemNanoMat, 2018, 4, 781-784.	1.5	10

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37	Quantum-Chemical Insights into the Self-Assembly of Carbon-Based Supramolecular Complexes. Molecules, 2018, 23, 118.	1.7	9
38	Heteroatom Effect on Starâ€Shaped Holeâ€Transporting Materials for Perovskite Solar Cells. Advanced Functional Materials, 2018, 28, 1801734.	7.8	62
39	Isomerism effect on the photovoltaic properties of benzotrithiophene-based hole-transporting materials. Journal of Materials Chemistry A, 2017, 5, 8317-8324.	5.2	86
40	DLPNO-CCSD(T) scaled methods for the accurate treatment of large supramolecular complexes. Journal of Computational Chemistry, 2017, 38, 1869-1878.	1.5	26
41	Theoretical insights into the structural, electronic and optical properties of benzotrithiophene-based hole-transporting materials. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	6
42	Controlling the Hostâ€“Guest Interaction Mode through a Redox Stimulus. Angewandte Chemie - International Edition, 2017, 56, 16272-16276.	7.2	91
43	Non-covalent graphene nanobuds from mono- and tripodal binding motifs. Chemical Communications, 2017, 53, 12402-12405.	2.2	26
44	Highâ€Efficiency Perovskite Solar Cells Using Molecularly Engineered, Thiopheneâ€Rich, Holeâ€Transporting Materials: Influence of Alkyl Chain Length on Power Conversion Efficiency. Advanced Energy Materials, 2017, 7, 1601674.	10.2	125
45	Photophysical Properties of OligoÂ(phenylene ethynylene) Iridium(III) Complexes Functionalized with Metal-Anchoring Groups. European Journal of Inorganic Chemistry, 2016, 2016, 1851-1859.	1.0	5
46	Exciton Dynamics in Phthalocyanine Molecular Crystals. Journal of Physical Chemistry C, 2016, 120, 7987-7996.	1.5	27
47	Helical supramolecular polymerization of C₃-symmetric amides and retroamides: on the origin of cooperativity and handedness. Chemical Communications, 2016, 52, 6907-6910.	2.2	29
48	Relationship between Electron Affinity and Halfâ€Wave Reduction Potential: A Theoretical Study on Cyclic Electronâ€Acceptor Compounds. ChemPhysChem, 2016, 17, 3881-3890.	1.0	15
49	Conjugated Porphyrin Dimers: Cooperative Effects and Electronic Communication in Supramolecular Ensembles with C₆₀. Journal of the American Chemical Society, 2016, 138, 15359-15367.	6.6	49
50	Regimes of Exciton Transport in Molecular Crystals in the Presence of Dynamic Disorder. Advanced Functional Materials, 2016, 26, 2316-2325.	7.8	65
51	Synthesis and optoelectronic properties of chemically modified bi-fluorenylidenes. Journal of Materials Chemistry C, 2016, 4, 3798-3808.	2.7	15
52	Nonâ€Centrosymmetric Homochiral Supramolecular Polymers of Tetrahedral Subphthalocyanine Molecules. Angewandte Chemie, 2015, 127, 2573-2577.	1.6	17
53	The Nonlocal Correlation Density Functional VV10. Annual Reports in Computational Chemistry, 2015, 11, 37-102.	0.9	17
54	Accurate Treatment of Large Supramolecular Complexes by Double-Hybrid Density Functionals Coupled with Nonlocal van der Waals Corrections. Journal of Chemical Theory and Computation, 2015, 11, 932-939.	2.3	48

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55	Nonâ€Centrosymmetric Homochiral Supramolecular Polymers of Tetrahedral Subphthalocyanine Molecules. Angewandte Chemie - International Edition, 2015, 54, 2543-2547.	7.2	63
56	Dynamics of the Excitonic Coupling in Organic Crystals. Physical Review Letters, 2015, 114, 026402.	2.9	111
57	High Yield Ultrafast Intramolecular Singlet Exciton Fission in a Quinoidal Bithiophene. Journal of Physical Chemistry Letters, 2015, 6, 1375-1384.	2.1	106
58	A columnar liquid crystal with permanent polar order. Journal of Materials Chemistry C, 2015, 3, 985-989.	2.7	33
59	Unveiling the nature of supramolecular crown etherâ€“C60 interactions. Chemical Science, 2015, 6, 4426-4432.	3.7	37
60	Charge Dynamics in Organic Photovoltaic Materials: Interplay between Quantum Diffusion and Quantum Relaxation. Journal of Physical Chemistry C, 2015, 119, 14989-14998.	1.5	24
61	Excitonic couplings between molecular crystal pairs by a multistate approximation. Journal of Chemical Physics, 2015, 142, 164107.	1.2	23
62	A very general rate expression for charge hopping in semiconducting polymers. Journal of Chemical Physics, 2015, 142, 184105.	1.2	30
63	Metalâ€Atom Impact on the Selfâ€Assembly of Cupâ€andâ€Ball Metalloporphyrinâ€“Fullerene Conjugates. Angewandte Chemie - International Edition, 2015, 54, 1255-1260.	7.2	36
64	Electron Transfer in a Supramolecular Associate of a Fullerene Fragment. Angewandte Chemie - International Edition, 2014, 53, 2170-2175.	7.2	52
65	Tuning the Self-Assembly of Rectangular Amphiphilic Cruciforms. Langmuir, 2014, 30, 5957-5964.	1.6	6
66	Theoretical study of the benzoquinoneâ€“tetrathiafulvaleneâ€“benzoquinone triad in neutral and oxidized/reduced states. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	12
67	Exploiting Multivalent Nanoparticles for the Supramolecular Functionalization of Graphene with a Nonplanar Recognition Motif. Chemistry - A European Journal, 2013, 19, 9843-9848.	1.7	15
68	Nonlocal van der Waals Approach Merged with Double-Hybrid Density Functionals: Toward the Accurate Treatment of Noncovalent Interactions. Journal of Chemical Theory and Computation, 2013, 9, 3437-3443.	2.3	53
69	A bis(triazole)benzamide receptor for the complexation of halide anions and neutral carboxylic acid guests. Guest-controlled topicity and self-assembly. Organic and Biomolecular Chemistry, 2013, 11, 765-772.	1.5	13
70	Impact of the Synergistic Collaboration of Oligothiophene Bridges and Ruthenium Complexes on the Optical Properties of Dumbbellâ€Shaped Compounds. Chemistry - A European Journal, 2013, 19, 1476-1488.	1.7	9
71	Obtaining the lattice energy of the anthracene crystal by modern yet affordable first-principles methods. Journal of Chemical Physics, 2013, 138, 204304.	1.2	17
72	Tetrathiafulvaleneâ€Based Mixedâ€Valence Acceptorâ€“Donorâ€“Acceptor Triads: A Joint Theoretical and Experimental Approach. Chemistry - A European Journal, 2013, 19, 16656-16664.	1.7	13

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73	Carbonylâ€Functionalized Quaterthiophenes: A Study of the Vibrational Raman and Electronic Absorption/Emission Properties Guided by Theoretical Calculations. ChemPhysChem, 2012, 13, 168-176.	1.0	8
74	Bowl-shape electron donors with absorptions in the visible range of the solar spectrum and their supramolecular assemblies with C₆₀. Chemical Science, 2012, 3, 498-508.	3.7	42
75	Oligothienoacenes versus oligothiophenes: impact of ring fusion on the optical properties. Physical Chemistry Chemical Physics, 2011, 13, 1457-1465.	1.3	30
76	Ab Initio Modeling of Donorâ€“Acceptor Interactions and Charge-Transfer Excitations in Molecular Complexes: The Case of Terthiopheneâ€“Tetracyanoquinodimethane. Journal of Chemical Theory and Computation, 2011, 7, 2068-2077.	2.3	46
77	Functionalized pentacenes: a combined theoretical, Raman and UVâ€“Vis spectroscopic study. Theoretical Chemistry Accounts, 2011, 128, 521-530.	0.5	22
78	Diferrocenyl oligothiophene wires: Raman and quantum chemical study of valence-trapped cations. Journal of Chemical Physics, 2011, 135, 234705.	1.2	2
79	Neutral and Oxidized Triisopropylsilyl Endâ€Capped Oligothienoacenes: A Combined Electrochemical, Spectroscopic, and Theoretical Study. Chemistry - A European Journal, 2010, 16, 5481-5491.	1.7	25
80	FT Raman and DFT Study on a Series of Allâ€anti Oligothienoacenes Endâ€Capped with Triisopropylsilyl Groups. ChemPhysChem, 2009, 10, 3069-3076.	1.0	11
81	From linear quaterthiophene to sulflower: A comparative theoretical study. Computational and Theoretical Chemistry, 2009, 912, 27-31.	1.5	11
82	Aromaticity of Î±-Oligothiophenes and Equivalent Oligothienoacenes. Journal of Chemical Theory and Computation, 2009, 5, 1767-1775.	2.3	6