

Juan Aragón³

List of Publications by Year in descending order

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papers

2,148
citations

201385

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85
docs citations

85
times ranked

3276
citing authors

#	ARTICLE	IF	CITATIONS
1	High Efficiency Perovskite Solar Cells Using Molecularly Engineered, Thiophene-Rich, Hole-Transporting Materials: Influence of Alkyl Chain Length on Power Conversion Efficiency. <i>Advanced Energy Materials</i> , 2017, 7, 1601674.	10.2	125
2	Dynamics of the Excitonic Coupling in Organic Crystals. <i>Physical Review Letters</i> , 2015, 114, 026402.	2.9	111
3	High Yield Ultrafast Intramolecular Singlet Exciton Fission in a Quinoidal Bithiophene. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1375-1384.	2.1	106
4	Controlling the Host-Guest Interaction Mode through a Redox Stimulus. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 16272-16276.	7.2	91
5	Isomerism effect on the photovoltaic properties of benzotrithiophene-based hole-transporting materials. <i>Journal of Materials Chemistry A</i> , 2017, 5, 8317-8324.	5.2	86
6	Regimes of Exciton Transport in Molecular Crystals in the Presence of Dynamic Disorder. <i>Advanced Functional Materials</i> , 2016, 26, 2316-2325.	7.8	65
7	Non-Centrosymmetric Homochiral Supramolecular Polymers of Tetrahedral Subphthalocyanine Molecules. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 2543-2547.	7.2	63
8	Heteroatom Effect on Star-Shaped Hole-Transporting Materials for Perovskite Solar Cells. <i>Advanced Functional Materials</i> , 2018, 28, 1801734.	7.8	62
9	Nonlocal van der Waals Approach Merged with Double-Hybrid Density Functionals: Toward the Accurate Treatment of Noncovalent Interactions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3437-3443.	2.3	53
10	Electron Transfer in a Supramolecular Associate of a Fullerene Fragment. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 2170-2175.	7.2	52
11	Conjugated Porphyrin Dimers: Cooperative Effects and Electronic Communication in Supramolecular Ensembles with C ₆₀ . <i>Journal of the American Chemical Society</i> , 2016, 138, 15359-15367.	6.6	49
12	Accurate Treatment of Large Supramolecular Complexes by Double-Hybrid Density Functionals Coupled with Nonlocal van der Waals Corrections. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 932-939.	2.3	48
13	Ab Initio Modeling of Donor-Acceptor Interactions and Charge-Transfer Excitations in Molecular Complexes: The Case of Terthiophene-Tetracyanoquinodimethane. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2068-2077.	2.3	46
14	Dibenzoquinquethiophene- and Dibenzosexithiophene-Based Hole-Transporting Materials for Perovskite Solar Cells. <i>Chemistry of Materials</i> , 2019, 31, 6435-6442.	3.2	46
15	Hole transporting materials based on benzodithiophene and dithienopyrrole cores for efficient perovskite solar cells. <i>Journal of Materials Chemistry A</i> , 2018, 6, 5944-5951.	5.2	44
16	Decoding the Consequences of Increasing the Size of Self-Assembling Tricarboxamides on Chiral Amplification. <i>Journal of the American Chemical Society</i> , 2019, 141, 7463-7472.	6.6	44
17	Distance Matters: Biasing Mechanism, Transfer of Asymmetry, and Stereomutation in N-Annulated Perylene Bisimide Supramolecular Polymers. <i>Journal of the American Chemical Society</i> , 2021, 143, 13281-13291.	6.6	43
18	Bowl-shape electron donors with absorptions in the visible range of the solar spectrum and their supramolecular assemblies with C ₆₀ . <i>Chemical Science</i> , 2012, 3, 498-508.	3.7	42

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19	In Silico Molecular Engineering of Dysprosocenium-Based Complexes to Decouple Spin Energy Levels from Molecular Vibrations. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7678-7683.	2.1	39
20	Unveiling the nature of supramolecular crown etherâ€C60 interactions. <i>Chemical Science</i> , 2015, 6, 4426-4432.	3.7	37
21	Metalâ€Atom Impact on the Selfâ€Assembly of Cupâ€andâ€Ball Metalloporphyrinâ€Fullerene Conjugates. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 1255-1260.	7.2	36
22	A columnar liquid crystal with permanent polar order. <i>Journal of Materials Chemistry C</i> , 2015, 3, 985-989.	2.7	33
23	Dual-Mode Chiral Self-Assembly of Cone-Shaped Subphthalocyanine Aromatics. <i>Journal of the American Chemical Society</i> , 2020, 142, 21017-21031.	6.6	32
24	Oligothienoacenes versus oligothiophenes: impact of ring fusion on the optical properties. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 1457-1465.	1.3	30
25	A very general rate expression for charge hopping in semiconducting polymers. <i>Journal of Chemical Physics</i> , 2015, 142, 184105.	1.2	30
26	Hole-Transporting Materials for Perovskite Solar Cells Employing an Anthradithiophene Core. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 28214-28221.	4.0	30
27	Helical supramolecular polymerization of C₃-symmetric amides and retroamides: on the origin of cooperativity and handedness. <i>Chemical Communications</i> , 2016, 52, 6907-6910.	2.2	29
28	Exciton Dynamics in Phthalocyanine Molecular Crystals. <i>Journal of Physical Chemistry C</i> , 2016, 120, 7987-7996.	1.5	27
29	Saddle-like, Î€-conjugated, cyclooctatetrathiophene-based, hole-transporting material for perovskite solar cells. <i>Journal of Materials Chemistry C</i> , 2019, 7, 6656-6663.	2.7	27
30	DLPNO-CCSD(T) scaled methods for the accurate treatment of large supramolecular complexes. <i>Journal of Computational Chemistry</i> , 2017, 38, 1869-1878.	1.5	26
31	Non-covalent graphene nanobuds from mono- and tripodal binding motifs. <i>Chemical Communications</i> , 2017, 53, 12402-12405.	2.2	26
32	Neutral and Oxidized Triisopropylsilyl Endâ€Capped Oligothienoacenes: A Combined Electrochemical, Spectroscopic, and Theoretical Study. <i>Chemistry - A European Journal</i> , 2010, 16, 5481-5491.	1.7	25
33	Hierarchy of Asymmetry at Work: Chainâ€Dependent Helixâ€toâ€Helix Interactions in Supramolecular Polymers. <i>Chemistry - A European Journal</i> , 2018, 24, 2826-2831.	1.7	25
34	Charge Dynamics in Organic Photovoltaic Materials: Interplay between Quantum Diffusion and Quantum Relaxation. <i>Journal of Physical Chemistry C</i> , 2015, 119, 14989-14998.	1.5	24
35	Excitonic couplings between molecular crystal pairs by a multistate approximation. <i>Journal of Chemical Physics</i> , 2015, 142, 164107.	1.2	23
36	Functionalized pentacenes: a combined theoretical, Raman and UVâ€Vis spectroscopic study. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 521-530.	0.5	22

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37	Spectroscopic Analysis of Vibronic Relaxation Pathways in Molecular Spin Qubit [Ho(W ₅ O ₁₈) ₂] ⁹⁺ : Sparse Spectra Are Key. <i>Inorganic Chemistry</i> , 2021, 60, 14096-14104.	1.9	22
38	Ternary Organic Solar Cell with a Near-Infrared Absorbing Selenophene-Diketopyrrolopyrrole-Based Nonfullerene Acceptor and an Efficiency above 10%. <i>Solar Rrl</i> , 2020, 4, 1900471.	3.1	21
39	Tetrasubstituted Thieno[3,2- <i>b</i>]thiophenes as Hole-Transporting Materials for Perovskite Solar Cells. <i>Journal of Organic Chemistry</i> , 2020, 85, 224-233.	1.7	20
40	Obtaining the lattice energy of the anthracene crystal by modern yet affordable first-principles methods. <i>Journal of Chemical Physics</i> , 2013, 138, 204304.	1.2	17
41	Non-Centrosymmetric Homochiral Supramolecular Polymers of Tetrahedral Subphthalocyanine Molecules. <i>Angewandte Chemie</i> , 2015, 127, 2573-2577.	1.6	17
42	The Nonlocal Correlation Density Functional VV10. <i>Annual Reports in Computational Chemistry</i> , 2015, 11, 37-102.	0.9	17
43	Exploiting Multivalent Nanoparticles for the Supramolecular Functionalization of Graphene with a Nonplanar Recognition Motif. <i>Chemistry - A European Journal</i> , 2013, 19, 9843-9848.	1.7	15
44	Relationship between Electron Affinity and Half-Wave Reduction Potential: A Theoretical Study on Cyclic Electron-Acceptor Compounds. <i>ChemPhysChem</i> , 2016, 17, 3881-3890.	1.0	15
45	Synthesis and optoelectronic properties of chemically modified bi-fluorenylidenes. <i>Journal of Materials Chemistry C</i> , 2016, 4, 3798-3808.	2.7	15
46	Azatruxene-Based, Dumbbell-Shaped, Donor- π -Bridge-Donor Hole-Transporting Materials for Perovskite Solar Cells. <i>Chemistry - A European Journal</i> , 2020, 26, 11039-11047.	1.7	15
47	Influence of the <i>Z/E</i> Isomerism on the Pathway Complexity of a Squaramide-Based Macrocyclic. <i>Small</i> , 2021, 17, e2006133.	5.2	14
48	A bis(triazole)benzamide receptor for the complexation of halide anions and neutral carboxylic acid guests. Guest-controlled topicity and self-assembly. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 765-772.	1.5	13
49	Tetrathiafulvalene-Based Mixed-Valence Acceptor-Donor-Acceptor Triads: A Joint Theoretical and Experimental Approach. <i>Chemistry - A European Journal</i> , 2013, 19, 16656-16664.	1.7	13
50	Improving the Robustness of Organic Semiconductors through Hydrogen Bonding. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 8620-8630.	4.0	13
51	Theoretical study of the benzoquinone-tetrathiafulvalene-benzoquinone triad in neutral and oxidized/reduced states. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	12
52	Understanding the affinity of bis-exTTF macrocyclic receptors towards fullerene recognition. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 11670-11675.	1.3	12
53	FT Raman and DFT Study on a Series of All-anti Oligothienoacenes End-Capped with Trisopropylsilyl Groups. <i>ChemPhysChem</i> , 2009, 10, 3069-3076.	1.0	11
54	From linear quaterthiophene to sulflower: A comparative theoretical study. <i>Computational and Theoretical Chemistry</i> , 2009, 912, 27-31.	1.5	11

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55	Synergy of Axial and Point Chirality to Construct Helical <i>N</i> -Heterotriangulene-Based Supramolecular Polymers. <i>ChemNanoMat</i> , 2018, 4, 781-784.	1.5	10
56	Flipping Motion To Bias the Organized Supramolecular Polymerization of N-Heterotriangulenes. <i>Chemistry of Materials</i> , 2019, 31, 7024-7032.	3.2	10
57	Impact of the Synergistic Collaboration of Oligothiophene Bridges and Ruthenium Complexes on the Optical Properties of Dumbbell-Shaped Compounds. <i>Chemistry - A European Journal</i> , 2013, 19, 1476-1488.	1.7	9
58	Quantum-Chemical Insights into the Self-Assembly of Carbon-Based Supramolecular Complexes. <i>Molecules</i> , 2018, 23, 118.	1.7	9
59	Impact of Molecular Size and Shape on the Supramolecular Co-Assembly of Chiral Tricarboxamides: A Comparative Study. <i>Chemistry - A European Journal</i> , 2020, 26, 14700-14707.	1.7	9
60	Carbonyl-Functionalized Quaterthiophenes: A Study of the Vibrational Raman and Electronic Absorption/Emission Properties Guided by Theoretical Calculations. <i>ChemPhysChem</i> , 2012, 13, 168-176.	1.0	8
61	Effect of Substituents at Imide Positions on the Laser Performance of 1,7-Bay-Substituted Perylene-diimide Dyes. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12277-12288.	1.5	7
62	Selenophene-Based Hole-Transporting Materials for Perovskite Solar Cells. <i>ChemPlusChem</i> , 2021, 86, 1006-1013.	1.3	7
63	Binding Sites, Vibrations and Spin-Lattice Relaxation Times in Europium(II)-Based Metallofullerene Spin Qubits. <i>Chemistry - A European Journal</i> , 2021, 27, 13242-13248.	1.7	7
64	Aromaticity of $\hat{I}\pm$ -Oligothiophenes and Equivalent Oligothienoacenes. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1767-1775.	2.3	6
65	Tuning the Self-Assembly of Rectangular Amphiphilic Cruciforms. <i>Langmuir</i> , 2014, 30, 5957-5964.	1.6	6
66	Theoretical insights into the structural, electronic and optical properties of benzotrithiophene-based hole-transporting materials. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	6
67	Self-Assembly-Directed Organization of a Fullerene-Bisporphyrin into Supramolecular Giant Donut Structures for Excited-State Charge Stabilization. <i>Journal of the American Chemical Society</i> , 2021, 143, 11199-11208.	6.6	6
68	Supramolecular assembly of pyrene-tetrathiafulvalene hybrids on graphene: structure-property relationships and biosensing activity. <i>Journal of Materials Chemistry C</i> , 2021, 9, 10944-10951.	2.7	6
69	Improving the Long-Term Stability of Doped Spiro-Type Hole-Transporting Materials in Planar Perovskite Solar Cells. <i>Solar Rrl</i> , 2021, 5, 2100650.	3.1	6
70	Photophysical Properties of Oligo(phenylene ethynylene) Iridium(III) Complexes Functionalized with Metal-Anchoring Groups. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 1851-1859.	1.0	5
71	Bending Carbon Nanoforms for Supramolecular Recognition: A Topological Study on Hemifullerene-Based Aggregates. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1124-1137.	1.1	5
72	Minimizing geminate recombination losses in small-molecule-based organic solar cells. <i>Journal of Materials Chemistry C</i> , 2019, 7, 6641-6648.	2.7	5

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73	On the Structure and Chiral Aggregation of Liquid Crystalline Star-Shaped Triazines H-Bonded to Benzoic Acids. <i>Chemistry - A European Journal</i> , 2020, 26, 15313-15322.	1.7	5
74	Effect of molecular geometry and extended conjugation on the performance of hydrogen-bonded semiconductors in organic thin-film field-effect transistors. <i>Journal of Materials Chemistry C</i> , 2021, 9, 10819-10829.	2.7	5
75	Tuning the electronic properties and the planarity degree in the π -extended TTF series: the prominent role of heteroatoms. <i>Journal of Materials Chemistry C</i> , 2018, 6, 13190-13196.	2.7	4
76	Tuning the optical and electronic properties of perylene diimides through transversal core extension. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	3
77	Non-Planar and Flexible Hole-Transporting Materials from Bis-Xanthene and Bis-Thioxanthene Units for Perovskite Solar Cells. <i>Helvetica Chimica Acta</i> , 2019, 102, e1900056.	1.0	3
78	Enhanced electronic communication through a conjugated bridge in a porphyrin-fullerene donor-acceptor couple. <i>Journal of Materials Chemistry C</i> , 2021, 9, 10889-10898.	2.7	3
79	Charge-Separation and Charge-Recombination Rate Constants in a Donor-Acceptor Buckybowl-Based Supramolecular Complex: Multistate and Solvent Effects. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9982-9994.	1.1	3
80	Diferrocenyl oligothiophene wires: Raman and quantum chemical study of valence-trapped cations. <i>Journal of Chemical Physics</i> , 2011, 135, 234705.	1.2	2
81	Self-Assembly of Clicked Star-Shaped Triazines into Functional Nanostructures. <i>ChemNanoMat</i> , 2019, 5, 130-137.	1.5	2
82	Frontispiece: Hierarchy of Asymmetry at Work: Chain-Dependent Helix-to-Helix Interactions in Supramolecular Polymers. <i>Chemistry - A European Journal</i> , 2018, 24, .	1.7	0