JoaquÃ-n Calbo

List of Publications by Year
in descending order

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83	2,491	201385	233125
papers	citations	27 h-index	45 g-index

97	97	97	3783
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Tuning Azoheteroarene Photoswitch Performance through Heteroaryl Design. Journal of the American Chemical Society, 2017, 139, 1261-1274.	6.6	244
2	Redox-active metalâ€“organic frameworks for energy conversion and storage. Journal of Materials Chemistry A, 2019, 7, 16571-16597.	5.2	207
3	Arylazopyrazoles for Long-Term Thermal Energy Storage and Optically Triggered Heat Release below 0 Â°C. Journal of the American Chemical Society, 2020, 142, 8688-8695.	6.6	121
4	Accumulation of Deep Traps at Grain Boundaries in Halide Perovskites. ACS Energy Letters, 2019, 4, 1321-1327.	8.8	117
5	Nâ€Annulated Perylene Bisimides to Bias the Differentiation of Metastable Supramolecular Assemblies into Jâ€•and Hâ€Aggregates. Angewandte Chemie - International Edition, 2020, 59, 17517-17524.	7.2	72
6	Nonâ€Centrosymmetric Homochiral Supramolecular Polymers of Tetrahedral Subphthalocyanine Molecules. Angewandte Chemie - International Edition, 2015, 54, 2543-2547.	7.2	63
7	Breathing-Dependent Redox Activity in a Tetrathiafulvalene-Based Metalâ€“Organic Framework. Journal of the American Chemical Society, 2018, 140, 10562-10569.	6.6	62
8	Heteroatom Effect on Starâ€Shaped Holeâ€Transporting Materials for Perovskite Solar Cells. Advanced Functional Materials, 2018, 28, 1801734.	7.8	62
9	A combinatorial approach to improving the performance of azoarene photoswitches. Beilstein Journal of Organic Chemistry, 2019, 15, 2753-2764.	1.3	53
10	Electron Transfer in a Supramolecular Associate of a Fullerene Fragment. Angewandte Chemie - International Edition, 2014, 53, 2170-2175.	7.2	52
11	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
12	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
13	Intrinsic doping limit and defect-assisted luminescence in Cs₄PbBr₆. Journal of Materials Chemistry A, 2019, 7, 20254-20261.	5.2	48
14	Role of the Bridge in Photoinduced Electron Transfer in Porphyrinâ€“Fullerene Dyads. Chemistry - A European Journal, 2015, 21, 5814-5825.	1.7	45
15	Tuning the Electronic Properties of Nonplanar exTTF-Based Pushâ€“Pull Chromophores by Aryl Substitution. Journal of Organic Chemistry, 2012, 77, 10707-10717.	1.7	44
16	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
17	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
18	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

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19	Chemical Zâ^'E Isomer Switching of Arylazopyrazoles Using Acid. ChemPhotoChem, 2019, 3, 372-377.	1.5	39
20	Unveiling the nature of supramolecular crown etherâ€"C60 interactions. Chemical Science, 2015, 6, 4426-4432.	3.7	37
21	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
22	Dual-Mode Chiral Self-Assembly of Cone-Shaped Subphthalocyanine Aromatics. Journal of the American Chemical Society, 2020, 142, 21017-21031.	6.6	32
23	Nâ€Annulated Perylene Bisimides to Bias the Differentiation of Metastable Supramolecular Assemblies into Jâ€and Hâ€Aggregates. Angewandte Chemie, 2020, 132, 17670-17677.	1.6	32
24	Determination of association constants towards carbon nanotubes. Chemical Science, 2015, 6, 7008-7014.	3.7	30
25	Understanding Noncovalent Interactions of Small Molecules with Carbon Nanotubes. Chemistry - A European Journal, 2017, 23, 12909-12916.	1.7	30
26	Mono- and Tripodal Porphyrins: Investigation on the Influence of the Number of Pyrene Anchors in Carbon Nanotube and Graphene Hybrids. Journal of the American Chemical Society, 2020, 142, 1895-1903.	6.6	30
27	Hole-Transporting Materials for Perovskite Solar Cells Employing an Anthradithiophene Core. ACS Applied Materials & Interfaces, 2021, 13, 28214-28221.	4.0	30
28	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
29	Flexible Chirality in Selfâ€Assembled Nâ€Annulated Perylenedicarboxamides. Small, 2017, 13, 1603880.	5.2	29
30	Computational modeling of single- versus double-anchoring modes in di-branched organic sensitizers on TiO₂ surfaces: structural and electronic properties. Physical Chemistry Chemical Physics, 2014, 16, 4709-4719.	1.3	28
31	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
32	On the handedness of helical aggregates of C₃ tricarboxamides: a multichiroptical characterization. Chemical Communications, 2015, 51, 9781-9784.	2.2	26
33	DLPNO-CCSD(T) scaled methods for the accurate treatment of large supramolecular complexes. Journal of Computational Chemistry, 2017, 38, 1869-1878.	1.5	26
34	Non-covalent graphene nanobuds from mono- and tripodal binding motifs. Chemical Communications, 2017, 53, 12402-12405.	2.2	26
35	Semiconductor Porous Hydrogen-Bonded Organic Frameworks Based on Tetrathiafulvalene Derivatives. Journal of the American Chemical Society, 2022, 144, 9074-9082.	6.6	26
36	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

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37	Charge-transfer interactions between fullerenes and a mesoporous tetrathiafulvalene-based metalâ€“organic framework. Beilstein Journal of Nanotechnology, 2019, 10, 1883-1893.	1.5	24
38	Biomimetic oxidation of pyrene and related aromatic hydrocarbons. Unexpected electron accepting abilities of pyrenequinones. Chemical Communications, 2014, 50, 9372-9375.	2.2	22
39	Tetrathiafulvaleneâ€“Polychlorotriphenylmethyl Dyads: Influence of Bridge and Openâ€Shell Characteristics on Linear and Nonlinear Optical Properties. Chemistry - A European Journal, 2017, 23, 11067-11075.	1.7	21
40	Complexation and Electronic Communication between Corannulene-Based Buckybowls and a Curved Truxene-TTF Donor. Chemistry - A European Journal, 2017, 23, 3666-3673.	1.7	20
41	Efficient Light Harvesters Based on the 10-(1,3-Dithiol-2-ylidene)anthracene Core. Organic Letters, 2013, 15, 4166-4169.	2.4	18
42	Tuning the Optical Absorption of Sn-, Ge-, and Zn-Substituted Cs₂AgBiBr₆ Double Perovskites: Structural and Electronic Effects. Chemistry of Materials, 2021, 33, 8028-8035.	3.2	18
43	The Nonlocal Correlation Density Functional VV10. Annual Reports in Computational Chemistry, 2015, 11, 37-102.	0.9	17
44	Blue-emitting pyrene-based aggregates. Chemical Communications, 2015, 51, 10142-10145.	2.2	17
45	Structural Dynamics and Tunability for Colloidal Tin Halide Perovskite Nanostructures. Advanced Materials, 2022, 34, e2201353.	11.1	16
46	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
47	Synthesis and optoelectronic properties of chemically modified bi-fluorenylidenes. Journal of Materials Chemistry C, 2016, 4, 3798-3808.	2.7	15
48	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
49	The Role of Planarity versus Nonplanarity in the Electronic Communication of TCAQâ€Based Pushâ€“Pull Chromophores. ChemPlusChem, 2018, 83, 300-307.	1.3	14
50	Colloidal nano-MOFs nucleate and stabilize ultra-small quantum dots of lead bromide perovskites. Chemical Science, 2021, 12, 6129-6135.	3.7	14
51	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
52	Multivariate sodalite zeolitic imidazolate frameworks: a direct solvent-free synthesis. Chemical Science, 2022, 13, 842-847.	3.7	13
53	Theoretical study of the benzoquinoneâ€“tetrathiafulvaleneâ€“benzoquinone triad in neutral and oxidized/reduced states. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	12
54	Understanding the affinity of bis-exTTF macrocyclic receptors towards fullerene recognition. Physical Chemistry Chemical Physics, 2019, 21, 11670-11675.	1.3	12

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55	Supramolecular polymerization of electronically complementary linear motifs: anti-cooperativity by attenuated growth. Chemical Science, 2021, 13, 81-89.	3.7	11
56	Exploiting the Redox Activity of MIL-100(Fe) Carrier Enables Prolonged Carvacrol Antimicrobial Activity. ACS Applied Materials & Interfaces, 2022, 14, 10758-10768.	4.0	11
57	Ligand engineering in Cu(<scp>ii</scp>) paddle wheel metalâ€“organic frameworks for enhanced semiconductivity. Journal of Materials Chemistry A, 2020, 8, 13160-13165.	5.2	10
58	Quantum-Chemical Insights into the Self-Assembly of Carbon-Based Supramolecular Complexes. Molecules, 2018, 23, 118.	1.7	9
59	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
60	Hexakis-adducts of [60]fullerene as molecular scaffolds of polynuclear spin-crossover molecules. Chemical Science, 2021, 12, 757-766.	3.7	7
61	Selenopheneâ€Based Holeâ€Transporting Materials for Perovskite Solar Cells. ChemPlusChem, 2021, 86, 1006-1013.	1.3	7
62	Theoretical insights into the structural, electronic and optical properties of benzotrithiophene-based hole-transporting materials. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	6
63	Efficient Benzodithiophene/Benzothiadiazoleâ€Based nâ€Channel Charge Transporters. ChemPlusChem, 2017, 82, 1105-1111.	1.3	6
64	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
65	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
66	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
67	Dielsâ€“Alder reaction on perylenediimides: synthesis and theoretical study of core-expanded diimides. Organic Chemistry Frontiers, 2019, 6, 2860-2871.	2.3	5
68	Minimizing geminate recombination losses in small-molecule-based organic solar cells. Journal of Materials Chemistry C, 2019, 7, 6641-6648.	2.7	5
69	Selective CO 2 Sorption Using Compartmentalized Coordination Polymers with Discrete Voids**. Chemistry - A European Journal, 2021, 27, 4653-4659.	1.7	5
70	Rhodanine-based dyes absorbing in the entire visible spectrum. Organic Chemistry Frontiers, 2017, 4, 1024-1028.	2.3	4
71	Carbon Nanotubes Conjugated with Triazoleâ€Based Tetrathiafulvaleneâ€Type Receptors for C₆₀ Recognition. ChemPlusChem, 2019, 84, 730-739.	1.3	4
72	Theoretical insight on novel donor-acceptor exTTF-based dyes for dye-sensitized solar cells. Journal of Molecular Modeling, 2014, 20, 2188.	0.8	3

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73	Supramolecular polymer chemistry meets computational chemistry: theoretical simulations on advanced self-assembling chiral materials. Supramolecular Chemistry, 2018, 30, 876-890.	1.5	3
74	Tuning the optical and electronic properties of perylene diimides through transversal core extension. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	3
75	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
76	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
77	Optical Properties of DMA-Ï€-DCV Derivatives: A Theoretical Inspection under the DFT Microscope. Journal of Spectroscopy, 2016, 2016, 1-12.	0.6	2
78	Allocation of Ambipolar Charges on an Organic Diradical with a Vinyleneâ€“Phenylenediyne Bridge. Journal of Physical Chemistry Letters, 2021, 12, 6159-6164.	2.1	2
79	Through-space hopping transport in an iodine-doped perylene-based metalâ€“organic framework. Molecular Systems Design and Engineering, 2022, 7, 1065-1072.	1.7	2
80	Frontispiece: Hierarchy of Asymmetry at Work: Chainâ€Dependent Helixâ€toâ€Helix Interactions in Supramolecular Polymers. Chemistry - A European Journal, 2018, 24, .	1.7	0
81	Perovskite Solar Cells: Heteroatom Effect on Starâ€Shaped Holeâ€Transporting Materials for Perovskite Solar Cells (Adv. Funct. Mater. 31/2018). Advanced Functional Materials, 2018, 28, 1870217.	7.8	0
82	InnenrÃ¼cktitelbild: Nâ€Annulated Perylene Bisimides to Bias the Differentiation of Metastable Supramolecular Assemblies into Jâ€and Hâ€Aggregates (Angew. Chem. 40/2020). Angewandte Chemie, 2020, 132, 17911-17911.	1.6	0
83	High Power Irradiance Dependence of Charge Species Dynamics in Hybrid Perovskites and Kinetic Evidence for Transient Vibrational Stark Effect in Formamidinium. Nanomaterials, 2022, 12, 1616.	1.9	0