BegoÃ±a MiliÃ¡n-Medina

List of Publications by Year
in descending order

52 papers	2,982 citations	172457 29 h-index	175258 52 g-index
52 all docs	52 docs citations	52 times ranked	4079 citing authors

#	Article	IF	Citations
1	A White-Light-Emitting Molecule: Frustrated Energy Transfer between Constituent Emitting Centers. Journal of the American Chemical Society, 2009, 131, 14043-14049.	13.7	553
2	Highly Emissive H-Aggregates or Aggregation-Induced Emission Quenching? The Photophysics of All-Trans para-Distyrylbenzene. Journal of Physical Chemistry Letters, 2013, 4, 2686-2697.	4.6	238
3	Solid-state optical properties of linear polyconjugated molecules: Ï€-stack contra herringbone. Journal of Chemical Physics, 2005, 123, 144914.	3.0	187
4	Solid State Luminescence Enhancement in Ï€-Conjugated Materials: Unraveling the Mechanism beyond the Framework of AIE/AIEE. Journal of Physical Chemistry C, 2017, 121, 23166-23183.	3.1	157
5	Luminescence in Crystalline Organic Materials: From Molecules to Molecular Solids. Advanced Optical Materials, 2021, 9, 2002251.	7.3	146
6	Highly efficient organic photocatalysts discovered via a computer-aided-design strategy for visible-light-driven atom transfer radical polymerization. Nature Catalysis, 2018, 1, 794-804.	34.4	124
7	Quinonoid Oligothiophenes as Electron-Donor and Electron-Acceptor Materials. A Spectroelectrochemical and Theoretical Study. Journal of the American Chemical Society, 2002, 124, 12380-12388.	13.7	109
8	Computational design of low singletâ€“triplet gap all-organic molecules for OLED application. Organic Electronics, 2012, 13, 985-991.	2.6	92
9	Effect of fluorination on the electronic structure and optical excitations of Ï€-conjugated molecules. Journal of Chemical Physics, 2007, 126, 111101.	3.0	84
10	Stimulated Emission Properties of Sterically Modified Distyrylbenzene-Based H-Aggregate Single Crystals. Journal of Physical Chemistry Letters, 2013, 4, 1597-1602.	4.6	71
11	Electronic Structure and Charge-Transport Properties of Polythiophene Chains Containing Thienothiophene Units: A Joint Experimental and Theoretical Study. Chemistry of Materials, 2007, 19, 4949-4956.	6.7	63
12	Naphthalenediimide Polymers with Finely Tuned Inâ€Chain Ï€â€Conjugation: Electronic Structure, Film Microstructure, and Charge Transport Properties. Advanced Materials, 2016, 28, 9169-9174.	21.0	63
13	Stimulated Resonance Raman Scattering and Laser Oscillation in Highly Emissive Distyrylbenzeneâ€Based Molecular Crystals. Advanced Materials, 2012, 24, 6473-6478.	21.0	62
14	Computational engineering of low bandgap copolymers. Frontiers in Chemistry, 2013, 1, 35.	3.6	59
15	On the electron affinity of TCNQ. Chemical Physics Letters, 2004, 391, 148-151.	2.6	51
16	Ï€â€Conjugation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 513-524.	14.6	51
17	Spectroscopic and Theoretical Study of the Molecular and Electronic Structures of a Terthiophene-Based Quinodimethane. ChemPhysChem, 2004, 5, 529-539.	2.1	46
18	Counterion-Mediated Crossing of the Cyanine Limit in Crystals and Fluid Solution: Bond Length Alternation and Spectral Broadening Unveiled by Quantum Chemistry. Journal of the American Chemical Society, 2020, 142, 2835-2843.	13.7	45

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19	Spectroscopic signatures for planar equilibrium geometries in methyl-substituted oligothiophenes. Physical Chemistry Chemical Physics, 2009, 11, 984-990.	2.8	43
20	Magnetic Properties of Quinoidal Oligothiophenes: More Than Good Candidates for Ambipolar Organic Semiconductors?. Advanced Functional Materials, 2006, 16, 531-536.	14.9	42
21	Spectroscopic and Theoretical Study of Pushâ^'Pull Chromophores Containing Thiophene-Based Quinonoid Structures as Electron Spacers. Journal of Physical Chemistry B, 2003, 107, 12175-12183.	2.6	40
22	Inverted energy gap law for the nonradiative decay in fluorescent floppy molecules: larger fluorescence quantum yields for smaller energy gaps. Organic Chemistry Frontiers, 2019, 6, 1948-1954.	4.5	40
23	Energy Transfer at the Zeoliteâ€…L Boundaries: Towards Photoâ€•and Electroresponsive Materials. ChemPlusChem, 2014, 79, 45-57.	2.8	38
24	Independent Tuning of Electronic Levels in Pentacene by Siteâ€Specific Substitution. ChemPhysChem, 2008, 9, 1519-1523.	2.1	37
25	EDOT-Type Materials: Planar but Not Rigid. Journal of Physical Chemistry A, 2008, 112, 13282-13286.	2.5	36
26	Bent-core liquid crystalline cyanostilbenes: fluorescence switching and thermochromism. Physical Chemistry Chemical Physics, 2015, 17, 11715-11724.	2.8	33
27	Magnetic and Conductive Properties of Quinoidal Oligothiophenes. Chemistry of Materials, 2006, 18, 1539-1545.	6.7	32
28	Oligothienoacenes versus oligothiophenes: impact of ring fusion on the optical properties. Physical Chemistry Chemical Physics, 2011, 13, 1457-1465.	2.8	30
29	Tetrakis{[(pâ€dodecacarboranyl)methyl]stilbenyl}ethylene: A Luminescent Tetraphenylethylene (TPE) Core System. European Journal of Inorganic Chemistry, 2017, 2017, 4575-4580.	2.0	30
30	â€œThough It Be but Little, It Is Fierceâ€: Excited State Engineering of Conjugated Organic Materials by Fluorination. Journal of Physical Chemistry Letters, 2017, 8, 91-101.	4.6	29
31	Twistâ€Elasticityâ€Controlled Crystal Emission in Highly Luminescent Polymorphs of Cyanoâ€Substituted Distyrylbenzene (ĩ²DCS). Advanced Optical Materials, 2017, 5, 1700340.	7.3	29
32	Fluoro-functionalization of vinylene units in a polyarylenevinylene for polymer solar cells. Journal of Materials Chemistry A, 2013, 1, 715-727.	10.3	27
33	Effective conjugation in conjugated polymers with strongly twisted backbones: a case study on fluorinated MEHPPV. Journal of Materials Chemistry C, 2016, 4, 6900-6906.	5.5	27
34	Calculation of low bandgap homopolymers: Comparison of TD-DFT methods with experimental oligomer series. Chemical Physics Letters, 2016, 645, 169-173.	2.6	26
35	A theoretical study of neutral and reduced tetracyano-p-quinodimethane (TCNQ). Computational and Theoretical Chemistry, 2004, 709, 97-102.	1.5	25
36	Excited-state switching by per-fluorination of para-oligophenylenes. Journal of Chemical Physics, 2011, 135, 124509.	3.0	25

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37	Oligophenylenevinylenes in Spatially Confined Nanochannels: Monitoring Intermolecular Interactions by UV/Vis and Raman Spectroscopy. Advanced Functional Materials, 2008, 18, 915-921.	14.9	20
38	Theoretical Study of the Electronic Excited States of Tetracyanoethylene and Its Radical Anion. ChemPhysChem, 2005, 6, 503-510.	2.1	18
39	Excited-state non-radiative decay in stilbenoid compounds: an ab initio quantum-chemistry study on size and substituent effects. Physical Chemistry Chemical Physics, 2019, 21, 22429-22439.	2.8	18
40	Dynamics of guest molecules in PHTP inclusion compounds as probed by solid-state NMR and fluorescence spectroscopy. Physical Chemistry Chemical Physics, 2009, 11, 4996.	2.8	17
41	Excited state absorption spectra of dissolved and aggregated distyrylbenzene: A TD-DFT state and vibronic analysis. Journal of Chemical Physics, 2017, 147, 034903.	3.0	17
42	Theoretical study of the molecular structure and the stability of neutral and reduced tetracyanoethylene. Chemical Physics Letters, 2003, 375, 376-382.	2.6	16
43	Molecular resolution friction microscopy of Cu phthalocyanine thin films on dolomite (104) in water. Nanoscale, 2014, 6, 8334-8339.	5.6	14
44	Crossed 2D versus Slipped 1D Ï€â€Stacking in Polymorphs of Crystalline Organic Thin Films: Impact on the Electronic and Optical Response. Advanced Optical Materials, 2019, 7, 1900749.	7.3	13
45	Regio(ir)regular naphthalenediimide- and perylenediimide-bithiophene copolymers: how MO localization controls the bandgap. Journal of Materials Chemistry C, 2016, 4, 9405-9410.	5.5	12
46	UVâ€“Vis, IR, Raman and theoretical characterization of a novel quinoid oligothiophene molecular material. Journal of Molecular Structure, 2003, 651-653, 665-673.	3.6	10
47	Design principles of chemiluminescence (CL) chemodosimeter for self-signaling detection: luminol protective approach. RSC Advances, 2014, 4, 46488-46493.	3.6	9
48	Tuning of the electronic and photophysical properties of ladder-type quaterphenyl by selective methylene-bridge fluorination. Physical Chemistry Chemical Physics, 2016, 18, 16501-16508.	2.8	9
49	Assembly-Induced Bright-Light Emission from Solution-Processed Platinum(II) Inorganic Polymers. ACS Omega, 2019, 4, 10192-10204.	3.5	6
50	Â¿Conjugated? Copolymers from a Pechmann Dye Derivative. Macromolecular Chemistry and Physics, 2016, 217, 2068-2073.	2.2	5
51	Combined Spectroscopic and TDâ€DFT Analysis to Elucidate Substituent and Acidochromic Effects in Organic Dyes: A Case Study on Aminoâ€versus Nitroâ€Substituted 2,4â€Diphenylquinolines. ChemPhysChem, 2020, 21, 1797-1804.	2.1	5
52	Quantum-chemistry study of the ground and excited state absorption of distyrylbenzene: Multi vs single reference methods. Journal of Chemical Physics, 2022, 156, 044102.	3.0	3