BegoÃ±a MiliÃ¡n-Medina

List of Publications by Year
in descending order

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52	2,982	196777	198040
papers	citations	29 h-index	52 g-index

52	52	52	4572
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum-chemistry study of the ground and excited state absorption of distyrylbenzene: Multi vs single reference methods. Journal of Chemical Physics, 2022, 156, 044102.	1.2	3
2	Luminescence in Crystalline Organic Materials: From Molecules to Molecular Solids. Advanced Optical Materials, 2021, 9, 2002251.	3.6	146
3	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.	1.0	5
4	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.	6.6	45
5	Crossed 2D versus Slipped 1D Ïâ€Stacking in Polymorphs of Crystalline Organic Thin Films: Impact on the Electronic and Optical Response. Advanced Optical Materials, 2019, 7, 1900749.	3.6	13
6	Assembly-Induced Bright-Light Emission from Solution-Processed Platinum(II) Inorganic Polymers. ACS Omega, 2019, 4, 10192-10204.	1.6	6
7	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.	2.3	40
8	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.	1.3	18
9	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.	16.1	124
10	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.	2.1	29
11	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.	1.5	157
12	Twistâ€Elasticityâ€Controlled Crystal Emission in Highly Luminescent Polymorphs of Cyanoâ€Substituted Distyrylbenzene (Î²DCS). Advanced Optical Materials, 2017, 5, 1700340.	3.6	29
13	Excited state absorption spectra of dissolved and aggregated distyrylbenzene: A TD-DFT state and vibronic analysis. Journal of Chemical Physics, 2017, 147, 034903.	1.2	17
14	Tetrakis{[(pâ€dodecacarboranyl)methyl]stilbenyl}ethylene: A Luminescent Tetraphenylethylene (TPE) Core System. European Journal of Inorganic Chemistry, 2017, 2017, 4575-4580.	1.0	30
15	Tuning of the electronic and photophysical properties of ladder-type quaterphenyl by selective methylene-bridge fluorination. Physical Chemistry Chemical Physics, 2016, 18, 16501-16508.	1.3	9
16	Regio(ir)regular naphthalenediimide- and perylenediimide-bithiophene copolymers: how MO localization controls the bandgap. Journal of Materials Chemistry C, 2016, 4, 9405-9410.	2.7	12
17	Naphthalenediimide Polymers with Finely Tuned Inâ€Chain Ïâ€Conjugation: Electronic Structure, Film Microstructure, and Charge Transport Properties. Advanced Materials, 2016, 28, 9169-9174.	11.1	63
18	Â¿Conjugated? Copolymers from a Pechmann Dye Derivative. Macromolecular Chemistry and Physics, 2016, 217, 2068-2073.	1.1	5

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19	Effective conjugation in conjugated polymers with strongly twisted backbones: a case study on fluorinated MEHPPV. Journal of Materials Chemistry C, 2016, 4, 6900-6906.	2.7	27
20	Calculation of low bandgap homopolymers: Comparison of TD-DFT methods with experimental oligomer series. Chemical Physics Letters, 2016, 645, 169-173.	1.2	26
21	Bent-core liquid crystalline cyanostilbenes: fluorescence switching and thermochromism. Physical Chemistry Chemical Physics, 2015, 17, 11715-11724.	1.3	33
22	Energy Transfer at the Zeoliteâ€…L Boundaries: Towards Photoâ€•and Electroresponsive Materials. ChemPlusChem, 2014, 79, 45-57.	1.3	38
23	Design principles of chemiluminescence (CL) chemodosimeter for self-signaling detection: luminol protective approach. RSC Advances, 2014, 4, 46488-46493.	1.7	9
24	Molecular resolution friction microscopy of Cu phthalocyanine thin films on dolomite (104) in water. Nanoscale, 2014, 6, 8334-8339.	2.8	14
25	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.	2.1	238
26	Fluoro-functionalization of vinylene units in a polyarylenevinylene for polymer solar cells. Journal of Materials Chemistry A, 2013, 1, 715-727.	5.2	27
27	Stimulated Emission Properties of Sterically Modified Distyrylbenzene-Based H-Aggregate Single Crystals. Journal of Physical Chemistry Letters, 2013, 4, 1597-1602.	2.1	71
28	Computational engineering of low bandgap copolymers. Frontiers in Chemistry, 2013, 1, 35.	1.8	59
29	Stimulated Resonance Raman Scattering and Laser Oscillation in Highly Emissive Distyrylbenzeneâ€Based Molecular Crystals. Advanced Materials, 2012, 24, 6473-6478.	11.1	62
30	Ïâ€Conjugation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 513-524.	6.2	51
31	Computational design of low singletâ€“triplet gap all-organic molecules for OLED application. Organic Electronics, 2012, 13, 985-991.	1.4	92
32	Oligothienoacenes versus oligothiophenes: impact of ring fusion on the optical properties. Physical Chemistry Chemical Physics, 2011, 13, 1457-1465.	1.3	30
33	Excited-state switching by per-fluorination of para-oligophenylenes. Journal of Chemical Physics, 2011, 135, 124509.	1.2	25
34	A White-Light-Emitting Molecule: Frustrated Energy Transfer between Constituent Emitting Centers. Journal of the American Chemical Society, 2009, 131, 14043-14049.	6.6	553
35	Spectroscopic signatures for planar equilibrium geometries in methyl-substituted oligothiophenes. Physical Chemistry Chemical Physics, 2009, 11, 984-990.	1.3	43
36	Dynamics of guest molecules in PHTP inclusion compounds as probed by solid-state NMR and fluorescence spectroscopy. Physical Chemistry Chemical Physics, 2009, 11, 4996.	1.3	17

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37	Independent Tuning of Electronic Levels in Pentacene by Siteâ€Specific Substitution. ChemPhysChem, 2008, 9, 1519-1523.	1.0	37
38	Oligophenylenevinylenes in Spatially Confined Nanochannels: Monitoring Intermolecular Interactions by UV/Vis and Raman Spectroscopy. Advanced Functional Materials, 2008, 18, 915-921.	7.8	20
39	EDOT-Type Materials: Planar but Not Rigid. Journal of Physical Chemistry A, 2008, 112, 13282-13286.	1.1	36
40	Effect of fluorination on the electronic structure and optical excitations of Ï€-conjugated molecules. Journal of Chemical Physics, 2007, 126, 111101.	1.2	84
41	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.	3.2	63
42	Magnetic and Conductive Properties of Quinoidal Oligothiophenes. Chemistry of Materials, 2006, 18, 1539-1545.	3.2	32
43	Magnetic Properties of Quinoidal Oligothiophenes: More Than Good Candidates for Ambipolar Organic Semiconductors?. Advanced Functional Materials, 2006, 16, 531-536.	7.8	42
44	Theoretical Study of the Electronic Excited States of Tetracyanoethylene and Its Radical Anion. ChemPhysChem, 2005, 6, 503-510.	1.0	18
45	Solid-state optical properties of linear polyconjugated molecules: Ï€-stack contra herringbone. Journal of Chemical Physics, 2005, 123, 144914.	1.2	187
46	Spectroscopic and Theoretical Study of the Molecular and Electronic Structures of a Terthiophene-Based Quinodimethane. ChemPhysChem, 2004, 5, 529-539.	1.0	46
47	A theoretical study of neutral and reduced tetracyano-p-quinodimethane (TCNQ). Computational and Theoretical Chemistry, 2004, 709, 97-102.	1.5	25
48	On the electron affinity of TCNQ. Chemical Physics Letters, 2004, 391, 148-151.	1.2	51
49	Theoretical study of the molecular structure and the stability of neutral and reduced tetracyanoethylene. Chemical Physics Letters, 2003, 375, 376-382.	1.2	16
50	UVâ€“Vis, IR, Raman and theoretical characterization of a novel quinoid oligothiophene molecular material. Journal of Molecular Structure, 2003, 651-653, 665-673.	1.8	10
51	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.	1.2	40
52	Quinonoid Oligothiophenes as Electron-Donor and Electron-Acceptor Materials. A Spectroelectrochemical and Theoretical Study. Journal of the American Chemical Society, 2002, 124, 12380-12388.	6.6	109