

Begoña Milán-Molina

List of Publications by Year in descending order

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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	Quantum-chemistry study of the ground and excited state absorption of distyrylbenzene: Multi vs single reference methods. <i>Journal of Chemical Physics</i> , 2022, 156, 044102.	3.0	3
2	Luminescence in Crystalline Organic Materials: From Molecules to Molecular Solids. <i>Advanced Optical Materials</i> , 2021, 9, 2002251.	7.3	146
3	Combined Spectroscopic and TD-DFT Analysis to Elucidate Substituent and Acidochromic Effects in Organic Dyes: A Case Study on Amino- versus Nitro-Substituted 2,4-Diphenylquinolines. <i>ChemPhysChem</i> , 2020, 21, 1797-1804.	2.1	5
4	Counterion-Mediated Crossing of the Cyanine Limit in Crystals and Fluid Solution: Bond Length Alternation and Spectral Broadening Unveiled by Quantum Chemistry. <i>Journal of the American Chemical Society</i> , 2020, 142, 2835-2843.	13.7	45
5	Crossed 2D versus Slipped 1D π -Stacking in Polymorphs of Crystalline Organic Thin Films: Impact on the Electronic and Optical Response. <i>Advanced Optical Materials</i> , 2019, 7, 1900749.	7.3	13
6	Assembly-Induced Bright-Light Emission from Solution-Processed Platinum(II) Inorganic Polymers. <i>ACS Omega</i> , 2019, 4, 10192-10204.	3.5	6
7	Inverted energy gap law for the nonradiative decay in fluorescent floppy molecules: larger fluorescence quantum yields for smaller energy gaps. <i>Organic Chemistry Frontiers</i> , 2019, 6, 1948-1954.	4.5	40
8	Excited-state non-radiative decay in stilbenoid compounds: an <i>ab initio</i> quantum-chemistry study on size and substituent effects. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22429-22439.	2.8	18
9	Highly efficient organic photocatalysts discovered via a computer-aided-design strategy for visible-light-driven atom transfer radical polymerization. <i>Nature Catalysis</i> , 2018, 1, 794-804.	34.4	124
10	“Though It Be but Little, It Is Fierce” Excited State Engineering of Conjugated Organic Materials by Fluorination. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 91-101.	4.6	29
11	Solid State Luminescence Enhancement in π -Conjugated Materials: Unraveling the Mechanism beyond the Framework of AIE/AIEE. <i>Journal of Physical Chemistry C</i> , 2017, 121, 23166-23183.	3.1	157
12	Twist-Elasticity-Controlled Crystal Emission in Highly Luminescent Polymorphs of Cyano-Substituted Distyrylbenzene (π^2 DCS). <i>Advanced Optical Materials</i> , 2017, 5, 1700340.	7.3	29
13	Excited state absorption spectra of dissolved and aggregated distyrylbenzene: A TD-DFT state and vibronic analysis. <i>Journal of Chemical Physics</i> , 2017, 147, 034903.	3.0	17
14	Tetrakis[[(<i>p</i> -dodecacarboranyl)methyl]stilbenyl]ethylene: A Luminescent Tetraphenylethylene (TPE) Core System. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 4575-4580.	2.0	30
15	Tuning of the electronic and photophysical properties of ladder-type quaterphenyl by selective methylene-bridge fluorination. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 16501-16508.	2.8	9
16	Regio(ir)regular naphthalenediimide- and perylenediimide-bithiophene copolymers: how MO localization controls the bandgap. <i>Journal of Materials Chemistry C</i> , 2016, 4, 9405-9410.	5.5	12
17	Naphthalenediimide Polymers with Finely Tuned In-Chain π -Conjugation: Electronic Structure, Film Microstructure, and Charge Transport Properties. <i>Advanced Materials</i> , 2016, 28, 9169-9174.	21.0	63
18	λ -Conjugated? Copolymers from a Pechmann Dye Derivative. <i>Macromolecular Chemistry and Physics</i> , 2016, 217, 2068-2073.	2.2	5

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19	Effective conjugation in conjugated polymers with strongly twisted backbones: a case study on fluorinated MEHPPV. <i>Journal of Materials Chemistry C</i> , 2016, 4, 6900-6906.	5.5	27
20	Calculation of low bandgap homopolymers: Comparison of TD-DFT methods with experimental oligomer series. <i>Chemical Physics Letters</i> , 2016, 645, 169-173.	2.6	26
21	Bent-core liquid crystalline cyanostilbenes: fluorescence switching and thermochromism. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 11715-11724.	2.8	33
22	Energy Transfer at the Zeolite-L Boundaries: Towards Photo- and Electroresponsive Materials. <i>ChemPlusChem</i> , 2014, 79, 45-57.	2.8	38
23	Design principles of chemiluminescence (CL) chemodosimeter for self-signaling detection: luminol protective approach. <i>RSC Advances</i> , 2014, 4, 46488-46493.	3.6	9
24	Molecular resolution friction microscopy of Cu phthalocyanine thin films on dolomite (104) in water. <i>Nanoscale</i> , 2014, 6, 8334-8339.	5.6	14
25	Highly Emissive H-Aggregates or Aggregation-Induced Emission Quenching? The Photophysics of All-Trans <i>para</i> -Distyrylbenzene. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2686-2697.	4.6	238
26	Fluoro-functionalization of vinylene units in a polyarylenevinylene for polymer solar cells. <i>Journal of Materials Chemistry A</i> , 2013, 1, 715-727.	10.3	27
27	Stimulated Emission Properties of Sterically Modified Distyrylbenzene-Based H-Aggregate Single Crystals. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1597-1602.	4.6	71
28	Computational engineering of low bandgap copolymers. <i>Frontiers in Chemistry</i> , 2013, 1, 35.	3.6	59
29	Stimulated Resonance Raman Scattering and Laser Oscillation in Highly Emissive Distyrylbenzene-Based Molecular Crystals. <i>Advanced Materials</i> , 2012, 24, 6473-6478.	21.0	62
30	Conjugation. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 513-524.	14.6	51
31	Computational design of low singlet-triplet gap all-organic molecules for OLED application. <i>Organic Electronics</i> , 2012, 13, 985-991.	2.6	92
32	Oligothienoacenes versus oligothiophenes: impact of ring fusion on the optical properties. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 1457-1465.	2.8	30
33	Excited-state switching by per-fluorination of <i>para</i> -oligophenylenes. <i>Journal of Chemical Physics</i> , 2011, 135, 124509.	3.0	25
34	A White-Light-Emitting Molecule: Frustrated Energy Transfer between Constituent Emitting Centers. <i>Journal of the American Chemical Society</i> , 2009, 131, 14043-14049.	18.7	553
35	Spectroscopic signatures for planar equilibrium geometries in methyl-substituted oligothiophenes. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 984-990.	2.8	43
36	Dynamics of guest molecules in PHTP inclusion compounds as probed by solid-state NMR and fluorescence spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4996.	2.8	17

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37	Independent Tuning of Electronic Levels in Pentacene by Site-Specific Substitution. <i>ChemPhysChem</i> , 2008, 9, 1519-1523.	2.1	37
38	Oligophenylenevinylenes in Spatially Confined Nanochannels: Monitoring Intermolecular Interactions by UV/Vis and Raman Spectroscopy. <i>Advanced Functional Materials</i> , 2008, 18, 915-921.	14.9	20
39	EDOT-Type Materials: Planar but Not Rigid. <i>Journal of Physical Chemistry A</i> , 2008, 112, 13282-13286.	2.5	36
40	Effect of fluorination on the electronic structure and optical excitations of π -conjugated molecules. <i>Journal of Chemical Physics</i> , 2007, 126, 111101.	3.0	84
41	Electronic Structure and Charge-Transport Properties of Polythiophene Chains Containing Thienothiophene Units: A Joint Experimental and Theoretical Study. <i>Chemistry of Materials</i> , 2007, 19, 4949-4956.	6.7	63
42	Magnetic and Conductive Properties of Quinoidal Oligothiophenes. <i>Chemistry of Materials</i> , 2006, 18, 1539-1545.	6.7	32
43	Magnetic Properties of Quinoidal Oligothiophenes: More Than Good Candidates for Ambipolar Organic Semiconductors?. <i>Advanced Functional Materials</i> , 2006, 16, 531-536.	14.9	42
44	Theoretical Study of the Electronic Excited States of Tetracyanoethylene and Its Radical Anion. <i>ChemPhysChem</i> , 2005, 6, 503-510.	2.1	18
45	Solid-state optical properties of linear polyconjugated molecules: π -stack contra herringbone. <i>Journal of Chemical Physics</i> , 2005, 123, 144914.	3.0	187
46	Spectroscopic and Theoretical Study of the Molecular and Electronic Structures of a Terthiophene-Based Quinodimethane. <i>ChemPhysChem</i> , 2004, 5, 529-539.	2.1	46
47	A theoretical study of neutral and reduced tetracyano-p-quinodimethane (TCNQ). <i>Computational and Theoretical Chemistry</i> , 2004, 709, 97-102.	1.5	25
48	On the electron affinity of TCNQ. <i>Chemical Physics Letters</i> , 2004, 391, 148-151.	2.6	51
49	Theoretical study of the molecular structure and the stability of neutral and reduced tetracyanoethylene. <i>Chemical Physics Letters</i> , 2003, 375, 376-382.	2.6	16
50	UV-Vis, IR, Raman and theoretical characterization of a novel quinoid oligothiophene molecular material. <i>Journal of Molecular Structure</i> , 2003, 651-653, 665-673.	3.6	10
51	Spectroscopic and Theoretical Study of Push-Pull Chromophores Containing Thiophene-Based Quinonoid Structures as Electron Spacers. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12175-12183.	2.6	40
52	Quinonoid Oligothiophenes as Electron-Donor and Electron-Acceptor Materials. A Spectroelectrochemical and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2002, 124, 12380-12388.	13.7	109