Amedeo Capobianco

List of Publications by Year
in descending order

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64 papers	1,340 citations	279701 23 h-index	395590 33 g-index
71 all docs	71 docs citations	71 times ranked	1163 citing authors

#	Article	IF	Citations
1	An intramolecularly self-templated synthesis of macrocycles: self-filling effects on the formation of prismarenes. Chemical Science, 2021, 12, 9952-9961.	3.7	27
2	The First Highly Enantioselective Synthesis of 3-Sulfinyl-Substituted Isoindolinones Having Adjacent Carbon and Sulfur Stereocenters. Journal of Organic Chemistry, 2021, 86, 10630-10639.	1.7	7
3	The Time Scale of Electronic Resonance in Oxidized DNA as Modulated by Solvent Response: An MD/QM-MM Study. Molecules, 2021, 26, 5497.	1.7	5
4	Is Aromatic Nitration Spin Density Driven?. Chemistry, 2021, 3, 1286-1301.	0.9	4
5	Prismarenes: A New Class of Macrocyclic Hosts Obtained by Templation in a Thermodynamically Controlled Synthesis. Journal of the American Chemical Society, 2020, 142, 1752-1756.	6.6	112
6	Phototautomerism of triazolo-triazole scaffold. Journal of Molecular Structure, 2020, 1203, 127368.	1.8	4
7	Tautomeric and conformational switching in a new versatile N-rich heterocyclic ligand. Dalton Transactions, 2020, 49, 14452-14462.	1.6	7
8	Coherent Effects in Charge Transport in Molecular Wires: Toward a Unifying Picture of Long-Range Hole Transfer in DNA. Journal of Physical Chemistry Letters, 2020, 11, 7769-7775.	2.1	16
9	Unravelling the mechanism of the organocatalyzed aminolytic kinetic resolution of Î±-nitroepoxides: a theoretical study. Catalysis Science and Technology, 2020, 10, 1422-1430.	2.1	3
10	The Dynamics of Hole Transfer in DNA. Molecules, 2019, 24, 4044.	1.7	25
11	Direct Î±-Imination of N-Acyl Pyrazoles with Nitrosoarenes. Organic Letters, 2019, 21, 5305-5309.	2.4	7
12	Disentangling Electronic and Vibrational Effects in the Prediction of Band Shapes for Singletâ€“Triplet Transitions. Journal of Physical Chemistry C, 2019, 123, 14173-14179.	1.5	10
13	Transient and Enduring Electronic Resonances Drive Coherent Long Distance Charge Transport in Molecular Wires. Journal of Physical Chemistry Letters, 2019, 10, 1845-1851.	2.1	17
14	1,5,7â€Triazabicyclo[4.4.0]decâ€5â€ene (TBD) Triggered Diastereoselective [3+2] Cycloaddition of Azomethine Imines and Pyrazoleamides. Advanced Synthesis and Catalysis, 2019, 361, 1018-1022.	2.1	21
15	Hole Hopping Rates in Organic Semiconductors: A Second-Order Cumulant Approach. Journal of Chemical Theory and Computation, 2018, 14, 1594-1601.	2.3	31
16	An Anthracene-Incorporated [8]Cycloparaphenylene Derivative as an Emitter in Photon Upconversion. Journal of Organic Chemistry, 2018, 83, 220-227.	1.7	22
17	Synthesis, Optoelectronic, and Supramolecular Properties of a Calix[4]areneâ€“Cycloparaphenylene Hybrid Host. Organic Letters, 2018, 20, 7415-7418.	2.4	12
18	Solid State Selection between Nearly Isoenergetic Tautomeric Forms Driven by Right Hydrogen-Bonding Pairing. Crystal Growth and Design, 2018, 18, 6293-6301.	1.4	7

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19	Second-Order Cumulant Approach for the Evaluation of Anisotropic Hole Mobility in Organic Semiconductors. Journal of Physical Chemistry C, 2018, 122, 25849-25857.	1.5	29
20	Single-Stranded DNA Oligonucleotides Retain Rise Coordinates Characteristic of Double Helices. Journal of Physical Chemistry B, 2018, 122, 7978-7989.	1.2	12
21	Stereoselective organocatalytic sulfa-Michael reactions of aryl substituted Î±,Î²-unsaturated N-acyl pyrazoles. Organic Chemistry Frontiers, 2018, 5, 1967-1977.	2.3	8
22	Modeling DNA oxidation in water. Physical Chemistry Chemical Physics, 2017, 19, 13571-13578.	1.3	16
23	Solid State Separation and Isolation of Tautomers of Fused-Ring Triazolotriazoles. Journal of Organic Chemistry, 2017, 82, 5155-5161.	1.7	14
24	Diastereodivergent and Enantioselective Access to Spiroepoxides via Organocatalytic Epoxidation of Unsaturated Pyrazolones. Organic Letters, 2017, 19, 5030-5033.	2.4	42
25	Stereoselective amine-thiourea-catalysed sulfa-Michael/nitroaldol cascade approach to 3,4,5-substituted tetrahydrothiophenes bearing a quaternary stereocenter. Beilstein Journal of Organic Chemistry, 2016, 12, 643-647.	1.3	13
26	Asymmetric tandem hemiaminal-heterocyclization-aza-Mannich reaction of 2-formylbenzonitriles and amines using chiral phase transfer catalysis: an experimental and theoretical study. RSC Advances, 2016, 6, 31861-31870.	1.7	22
27	First-Principle Calculations of the Band Shapes of Singletâ€“Triplet Transitions. Journal of Physical Chemistry C, 2016, 120, 24605-24614.	1.5	8
28	Absorption Band Shapes of a Pushâ€“Pull Dye Approaching the Cyanine Limit: A Challenging Case for First Principle Calculations. Journal of Physical Chemistry A, 2016, 120, 5581-5589.	1.1	31
29	The association constant of 5â€²,8-cyclo-2â€²-deoxyguanosine with cytidine. Frontiers in Chemistry, 2015, 3, 22.	1.8	4
30	Electrochemically Induced N-Alkylation of Chiral 2-(Methylsulfinyl) 1H-Benzimidazole. Synthetic Communications, 2015, 45, 1783-1791.	1.1	2
31	One-pot highly diastereoselective annulation to N-unprotected tetrasubstituted 2-pyrrolines. Green Chemistry, 2015, 17, 2137-2140.	4.6	18
32	Hole delocalization over adenine tracts in single stranded DNA oligonucleotides. Physical Chemistry Chemical Physics, 2015, 17, 4750-4756.	1.3	27
33	First Principle Analysis of Charge Dissociation and Charge Recombination Processes in Organic Solar Cells. Journal of Physical Chemistry C, 2015, 119, 18870-18876.	1.5	8
34	Vibronic couplings and coherent electron transfer in bridged systems. Physical Chemistry Chemical Physics, 2015, 17, 30937-30945.	1.3	23
35	Proton induced tautomeric switching in N-rich aromatics with tunable acid-base character. Journal of Molecular Structure, 2015, 1093, 119-124.	1.8	13
36	Delocalized Hole Domains in Guanine-Rich DNA Oligonucleotides. Journal of Physical Chemistry B, 2015, 119, 5462-5466.	1.2	33

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37	DFT predictions of the oxidation potential of organic dyes for opto-electronic devices. Computational and Theoretical Chemistry, 2015, 1070, 68-75.	1.1	11
38	The oxidization potential of AA steps in single strand DNA oligomers. RSC Advances, 2014, 4, 47887-47893.	1.7	18
39	Hole hopping rates in single strand oligonucleotides. Chemical Physics, 2014, 440, 25-30.	0.9	15
40	Franckâ€“Condon factorsâ€”Computational approaches and recent developments. Canadian Journal of Chemistry, 2013, 91, 495-504.	0.6	52
41	Stacking Interactions between Adenines in Oxidized Oligonucleotides. Journal of Physical Chemistry B, 2013, 117, 8947-8953.	1.2	24
42	Proton transfer in oxidized adenosine self-aggregates. Journal of Chemical Physics, 2013, 139, 145101.	1.2	16
43	Molecular hyperpolarizabilities of pushâ€“pull chromophores: A comparison between theoretical and experimental results. Chemical Physics, 2013, 411, 11-16.	0.9	28
44	Detection of an ylide intermediate in the electrochemically-induced Stevens rearrangement of an ammonium salt by in situ UVâ€“vis spectroelectrochemistry. Electrochimica Acta, 2013, 92, 446-451.	2.6	5
45	Ring to open-chain transformation induced by selective metal coordination in a new dithiocarbazate ligand. Inorganica Chimica Acta, 2013, 404, 29-33.	1.2	11
46	Electro-optical properties from CC2 Calculations: A comparison between theoretical and experimental results. Chemical Physics Letters, 2013, 580, 126-129.	1.2	14
47	Polar crystals in imines of 4-hydroxybenzohydrazide: a comparison between racemic and enantiomorphic crystals. CrystEngComm, 2013, 15, 3318.	1.3	15
48	Tautomerism in the Fused Nâ€Rich TriÂazolotriazole Heterocyclic System. European Journal of Organic Chemistry, 2013, 2013, 3721-3728.	1.2	26
49	Franckâ€“Condon factors in curvilinear coordinates: the photoelectron spectrum of ammonia. Highlights in Theoretical Chemistry, 2013, , 207-216.	0.0	0
50	On the Mechanism of Asymmetric Epoxidation of Enones Catalyzed by Î±,Î±â€‹scp›L‹/scp›â€Diarylprolinols: A Theoretical Insight. Advanced Synthesis and Catalysis, 2012, 354, 2789-2796.	2.1	34
51	A SAPT Study of the H2O X2 Complexes; X = H, N and F. , 2012, , .		0
52	Generating Function Approach to the Calculation of Spectral Band Shapes of Free-Base Chlorin Including Duschinsky and Herzbergâ€“Teller Effects. Journal of Physical Chemistry A, 2012, 116, 9934-9940.	1.1	78
53	Potential energy surfaces for interactions of H2O with H2, N2 and O2: A hyperspherical harmonics representation, and a minimal model for the H2Oâ€“rare-gas-atom systems. Computational and Theoretical Chemistry, 2012, 990, 53-61.	1.1	47
54	A series of compounds forming polar crystals and showing single-crystal-to-single-crystal transitions between polar phases. CrystEngComm, 2012, 14, 2645.	1.3	45

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55	Tuning Wavefunction Mixing in Pushâ€“Pull Molecules: From Neutral to Zwitterionic Compounds. European Journal of Organic Chemistry, 2012, 2012, 2980-2989.	1.2	28
56	Franckâ€“Condon factors in curvilinear coordinates: the photoelectron spectrum of ammonia. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	38
57	Enantioselective Conjugate Addition of Malononitrile to Chalcones Promoted by Î±,Î±â€<scp>L</scp>â€Diaryl Prolinols: Noncovalent versus Covalent Catalysis?. European Journal of Organic Chemistry, 2011, 2011, 1922-1931.	1.2	25
58	Competitive H-bonding synthons in organic hydrazides. CrystEngComm, 2010, 12, 1186-1193.	1.3	16
59	Photoelectron Spectrum of Ammonia, a Test Case for the Calculation of Franckâ^'Condon Factors in Molecules Undergoing Large Geometrical Displacements upon Photoionization. Journal of Physical Chemistry A, 2009, 113, 14831-14837.	1.1	36
60	Pushâ€“Pull Azoâ€Chromophores Containing Two Fused Pentatomic Heterocycles and Their Nonlinear Optical Properties. European Journal of Organic Chemistry, 2009, 2009, 3535-3543.	1.2	18
61	The Chargeâ€Transfer Band of an Oxidized Watsonâ€“Crick Guanosineâ€“Cytidine Complex. Angewandte Chemie - International Edition, 2009, 48, 9526-9528.	7.2	28
62	The Oxidation Potential of Adenosine and Adenosine-Thymidine Base Pair in Chloroform Solution. Journal of the American Chemical Society, 2007, 129, 15347-15353.	6.6	34
63	MO-LCAO approach and ab initio computations. International Journal of Quantum Chemistry, 2006, 106, 2014-2025.	1.0	0
64	Proton Assisted Electron Transfer. Advances in Quantum Chemistry, 2000, 36, 301-322.	0.4	10