Simona Fantacci

List of Publications by Year
in descending order

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Version: 2024-02-01

109 papers	10,766 citations	50170 46 h-index	30010 103 g-index
110 all docs	110 docs citations	110 times ranked	9860 citing authors

#	Article	IF	Citations
1	Modelling the Interaction between Carboxylic Acids and Zinc Oxide: Insight into Degradation of ZnO Pigments. Molecules, 2022, 27, 3362.	1.7	1
2	New insights into the deterioration of TiO2 based oil paints: the effects of illumination conditions and surface interactions. Heritage Science, 2022, 10, .	1.0	5
3	Influence of surfactants in improving degradation of polluting dyes photocatalyzed by TiO2 in aqueous dispersion. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 418, 113342.	2.0	9
4	First member of an appealing class of cyclometalated 1,3-di-(2-pyridyl)benzene platinum(<scp>ii</scp>) complexes for solution-processable OLEDs. Journal of Materials Chemistry C, 2020, 8, 7873-7881.	2.7	18
5	A combined theoretical and experimental investigation of the electronic and vibrational properties of red lead pigment. Journal of Cultural Heritage, 2020, 46, 374-381.	1.5	5
6	A Chiral Bis(salicylaldiminato)zinc(II) Complex with Second-Order Nonlinear Optical and Luminescent Properties in Solution. Inorganics, 2020, 8, 25.	1.2	18
7	Perylenetetracarboxy-3,4:9,10-diimide derivatives with large two-photon absorption activity. New Journal of Chemistry, 2019, 43, 1885-1893.	1.4	7
8	Ab Initio Modeling of Solar Cell Dye Sensitizers: The Hunt for Red Photons Continues. European Journal of Inorganic Chemistry, 2019, 2019, 743-750.	1.0	7
9	Novel cyclometallated 5-Ï€-delocalized donor-1,3-di(2-pyridyl)benzene platinum(<scp>ii</scp>) complexes with good second-order nonlinear optical properties. Dalton Transactions, 2019, 48, 202-208.	1.6	12
10	Interface Electrostatics of Solid-State Dye-Sensitized Solar Cells: A Joint Drift-Diffusion and Density Functional Theory Study. Journal of Physical Chemistry C, 2019, 123, 14955-14963.	1.5	7
11	Towards efficient sustainable full-copper dye-sensitized solar cells. Dalton Transactions, 2019, 48, 9703-9711.	1.6	43
12	Design of cyclometallated 5-Ï€-delocalized donor-1,3-di(2-pyridyl)benzene platinum(II) complexes with second-order nonlinear optical properties. Polyhedron, 2018, 140, 74-77.	1.0	17
13	Zur Photochemie von KÃ¼nstlerfarben: Strategien zur Verhinderung von FarbverÃnderungen in Kunstwerken. Angewandte Chemie, 2018, 130, 7447-7457.	1.6	1
14	Photochemistry of Artistsâ€™ Dyes and Pigments: Towards Better Understanding and Prevention of Colour Change in Works of Art. Angewandte Chemie - International Edition, 2018, 57, 7324-7334.	7.2	42
15	From Blue to Green: Fine-Tuning of Photoluminescence and Electrochemiluminescence in Bifunctional Organic Dyes. Journal of the American Chemical Society, 2017, 139, 2060-2069.	6.6	73
16	Designing Squaraines to Control Charge Injection and Recombination Processes in NiOâ€based Dyeâ€Sensitized Solar Cells. ChemSusChem, 2017, 10, 2385-2393.	3.6	20
17	Tuning the dipolar second-order nonlinear optical properties of 5-Ï€-delocalized-donor-1,3-di(2-pyridyl)benzenes, related cyclometallated platinum(<scp>ii</scp>) complexes and methylated salts. Dalton Transactions, 2017, 46, 1179-1185.	1.6	10
18	Novel Fullerene Platinum Alkynyl Complexes with High Second-Order Nonlinear Optical Properties as a Springboard for NLO-Active Polymer Films. Organometallics, 2016, 35, 1015-1021.	1.1	20

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19	Structural and electronic properties of the PbCrO₄ chrome yellow pigment and of its light sensitive sulfate-substituted compounds. RSC Advances, 2016, 6, 36336-36344.	1.7	21
20	Cobalt Polypyridyl Complexes as Transparent Solutionâ€Processable Solidâ€State Charge Transport Materials. Advanced Energy Materials, 2016, 6, 1600874.	10.2	25
21	Geometrical and energetical structural changes in organic dyes for dye-sensitized solar cells probed using photoelectron spectroscopy and DFT. Physical Chemistry Chemical Physics, 2016, 18, 252-260.	1.3	28
22	DFT/TDDFT investigation on the UV-vis absorption and fluorescence properties of alizarin dye. Physical Chemistry Chemical Physics, 2015, 17, 6374-6382.	1.3	47
23	A computational approach to the electronic, optical and acidâ€"base properties of Ru(II) dyes for photoelectrochemical solar cells applications. Polyhedron, 2014, 82, 88-103.	1.0	3
24	Time-Dependent Density Functional Theory Modeling of Spinâ€"Orbit Coupling in Ruthenium and Osmium Solar Cell Sensitizers. Journal of Physical Chemistry C, 2014, 118, 17067-17078.	1.5	51
25	Impact of Spinâ€"Orbit Coupling on Photocurrent Generation in Ruthenium Dye-Sensitized Solar Cells. Journal of Physical Chemistry Letters, 2014, 5, 375-380.	2.1	31
26	Theoretical Studies on Anatase and Less Common TiO₂ Phases: Bulk, Surfaces, and Nanomaterials. Chemical Reviews, 2014, 114, 9708-9753.	23.0	367
27	Electronic and Optical Properties of Dye-Sensitized TiO2 Interfaces. Topics in Current Chemistry, 2014, 347, 1-45.	4.0	18
28	Design of Ru(II) sensitizers endowed by three anchoring units for adsorption mode and light harvesting optimization. Thin Solid Films, 2014, 560, 86-93.	0.8	9
29	Protic Ionic Liquids as p-Dopant for Organic Hole Transporting Materials and Their Application in High Efficiency Hybrid Solar Cells. Journal of the American Chemical Society, 2013, 135, 13538-13548.	6.6	167
30	A Simple Synthetic Route to Obtain Pure Transâ€Ruthenium(II) Complexes for Dyeâ€Sensitized Solar Cell Applications. ChemSusChem, 2013, 6, 2170-2180.	3.6	27
31	Modeling Excited States and Alignment of Energy Levels in Dye-Sensitized Solar Cells: Successes, Failures, and Challenges. Journal of Physical Chemistry C, 2013, 117, 3685-3700.	1.5	137
32	An investigation on the second order nonlinear optical response of tris-cyclometallated Ir(<scp>iii</scp>) complexes with variously substituted 2-phenylpyridines. Dalton Transactions, 2013, 42, 155-159.	1.6	19
33	Role of Hot Singlet Excited States in Charge Generation at the Black Dye/TiO₂ Interface. ACS Applied Materials & Interfaces, 2013, 5, 4334-4339.	4.0	25
34	Tuning the Dipolar Secondâ€Order Nonlinear Optical Properties of Cyclometalated Platinum(II) Complexes with Tridentate N^C^N Binding Ligands. Chemistry - A European Journal, 2013, 19, 9875-9883.	1.7	48
35	Everything you always wanted to Know about Black Dye (but Were Afraid to Ask): A DFT/TDDFT Investigation. Chimia, 2013, 67, 121-128.	0.3	19
36	Computational Investigations on Organic Sensitizers for Dye-Sensitized Solar Cell. Current Organic Synthesis, 2012, 9, 215-232.	0.7	20

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37	Discoloration of the smalt pigment: experimental studies and ab initio calculations. Journal of Analytical Atomic Spectrometry, 2012, 27, 1941.	1.6	21
38	New [(D-terpyridine)-Ru-(D or A-terpyridine)][4-EtPhCO2]2 complexes (D = electron donor group; A =) Tj ETQq0 0 0 rgBT /Overlock 10 T Transactions, 2012, 41, 6707.	1.6	17
39	Influence of Donor Groups of Organic Dâ˜Ï€â€“A Dyes on Open-Circuit Voltage in Solid-State Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2012, 116, 1572-1578.	1.5	69
40	DFT/TDDFT investigation of the stepwise deprotonation in tetracycline: pKa assignment and UVâ€“vis spectroscopy. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	16
41	Computational Spectroscopy Characterization of the Species Involved in Dye Oxidation and Regeneration Processes in Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2011, 115, 18863-18872.	1.5	22
42	Electronic and Optical Properties of the Spiro-MeOTAD Hole Conductor in Its Neutral and Oxidized Forms: A DFT/TDDFT Investigation. Journal of Physical Chemistry C, 2011, 115, 23126-23133.	1.5	145
43	Panchromatic ruthenium sensitizer based on electron-rich heteroarylvinylene Ï€-conjugated quaterpyridine for dye-sensitized solar cells. Dalton Transactions, 2011, 40, 234-242.	1.6	57
44	A computational approach to the electronic and optical properties of Ru(II) and Ir(III) polypyridyl complexes: Applications to DSC, OLED and NLO. Coordination Chemistry Reviews, 2011, 255, 2704-2726.	9.5	161
45	Absorption Spectra and Excited State Energy Levels of the N719 Dye on TiO₂ in Dye-Sensitized Solar Cell Models. Journal of Physical Chemistry C, 2011, 115, 8825-8831.	1.5	222
46	Simulating Dye-Sensitized TiO₂ Heterointerfaces in Explicit Solvent: Absorption Spectra, Energy Levels, and Dye Desorption. Journal of Physical Chemistry Letters, 2011, 2, 813-817.	2.1	98
47	Cyclometalated Iridium(III) Complexes Based on Phenyl-Imidazole Ligand. Inorganic Chemistry, 2011, 50, 451-462.	1.9	98
48	pHâ€Sensitive Bis(2,2â€²:6â€²,2"â€terpyridine)ruthenium(II) Complexes â€“ A DFT/TDDFT Investigation of Their Spectroscopic Properties. European Journal of Inorganic Chemistry, 2011, 2011, 1605-1613.	1.0	12
49	Organic dyes incorporating low-band-gap chromophores based on Ï€-extended benzothiadiazole for dye-sensitized solar cells. Dyes and Pigments, 2011, 91, 192-198.	2.0	160
50	Theoretical and experimental investigation on the spectroscopic properties of indigo dye. Journal of Molecular Structure, 2011, 993, 43-51.	1.8	61
51	Ab Initio Determination of Ground and Excited State Oxidation Potentials of Organic Chromophores for Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2010, 114, 22742-22750.	1.5	135
52	A Joint Experimental and Theoretical Investigation on Nonlinear Optical (NLO) Properties of a New Class of Pushâ€“Pull Spirobifluorene Compounds. European Journal of Organic Chemistry, 2010, 2010, 4004-4016.	1.2	29
53	Cyclometalated Ir^{III} Complexes with Substituted 1,10â€Phenanthrolines: A New Class of Efficient Cationic Organometallic Secondâ€Order NLO Chromophores. Chemistry - A European Journal, 2010, 16, 4814-4825.	1.7	65
54	Complexation of apigenin and luteolin in weld lake: a DFT/TDDFT investigation. Physical Chemistry Chemical Physics, 2010, 12, 6672.	1.3	38

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55	Computational Chemistry Meets Cultural Heritage: Challenges and Perspectives. Accounts of Chemical Research, 2010, 43, 802-813.	7.6	48
56	First-Principles Modeling of the Adsorption Geometry and Electronic Structure of Ru(II) Dyes on Extended TiO₂ Substrates for Dye-Sensitized Solar Cell Applications. Journal of Physical Chemistry C, 2010, 114, 6054-6061.	1.5	224
57	Highly stable 7-N,N-dibutylamino-2-azaphenanthrene and 8-N,N-dibutylamino-2-azachrysene as a new class of second order NLO-active chromophores. Chemical Communications, 2010, 46, 8374.	2.2	9
58	An inconvenient influence of iridium(iii) isomer on OLED efficiency. Dalton Transactions, 2010, 39, 8914.	1.6	38
59	Luminescent cyclometallated Ir(iii) and Pt(ii) complexes with Î²-diketonate ligands as highly active second-order NLO chromophores. Chemical Communications, 2010, 46, 2414.	2.2	64
60	Stabilization through p-dimethylaminobenzaldehyde of a new NLO-active phase of [E-4-(4-dimethylaminostyryl)-1-methylpyridinium] iodide: synthesis, structural characterization and theoretical investigation of its electronic properties. Journal of Materials Chemistry, 2010, 20, 7652.	6.7	15
61	Panchromatic Crossâ€Substituted Squaraines for Dyeâ€Sensitized Solar Cell Applications. ChemSusChem, 2009, 2, 621-624.	3.6	51
62	Spectroscopic properties of cyclometallated iridium complexes by TDDFT. Computational and Theoretical Chemistry, 2009, 914, 74-86.	1.5	31
63	Cationic cyclometallated iridium(III) complexes with substituted 1,10-phenanthrolines: the role of the cyclometallated moiety on this new class of complexes with interesting luminescent and second order non linear optical properties. Journal of Materials Science: Materials in Electronics, 2009, 20, 460-464.	1.1	17
64	An EFISH, Theoretical, and PGSE NMR Investigation on the Relevant Role of Aggregation on the Second Order Response in CHCl3 of the Pushâ˜Pull Chromophores [5-[[4â€²-(Dimethylamino)phenyl]ethynyl]-15-[(4â€²â€²-nitrophenyl)ethynyl]-10,20-diphenylporphyrinate] M(II) (M)Tj ETQq0 0 0 rgBT	1.5	23
65	White-light phosphorescence emission from a single molecule: application to OLED. Chemical Communications, 2009, , 4672.	2.2	92
66	High Open-Circuit Voltage Solid-State Dye-Sensitized Solar Cells with Organic Dye. Nano Letters, 2009, 9, 2487-2492.	4.5	228
67	Absorption and Emission of the Apigenin and Luteolin Flavonoids: A TDDFT Investigation. Journal of Physical Chemistry A, 2009, 113, 15118-15126.	1.1	77
68	Theoretical investigation of the structural and electronic properties of luteolin, apigenin and their deprotonated species. Computational and Theoretical Chemistry, 2008, 868, 12-21.	1.5	14
69	Acidâ€"base chemistry of luteolin and its methyl-ether derivatives: A DFT and ab initio investigation. Chemical Physics Letters, 2008, 462, 313-317.	1.2	14
70	The role of 5-R-1,10-phenanthroline (R=CH3, NO2) on the emission properties and second-order NLO response of cationic Ir(III) organometallic chromophores. Inorganica Chimica Acta, 2008, 361, 4070-4076.	1.2	41
71	Alignment of the dyeâ€™s molecular levels with the TiO₂band edges in dye-sensitized solar cells: a DFTâ€"TDDFT study. Nanotechnology, 2008, 19, 424002.	1.3	263
72	Theoretical Study of the Structural and Electronic Properties of Luteolin and Apigenin Dyes. Lecture Notes in Computer Science, 2008, , 1141-1155.	1.0	2

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73	Electron-rich heteroaromatic conjugated bipyridine based ruthenium sensitizer for efficient dye-sensitized solar cells. Chemical Communications, 2008, , 5318.	2.2	107
74	Synthesis, Characterization, and DFT/TD-DFT Calculations of Highly Phosphorescent Blue Light-Emitting Anionic Iridium Complexes. Inorganic Chemistry, 2008, 47, 980-989.	1.9	222
75	Theoretical Investigations of the Effects of J-Aggregation on the Linear and Nonlinear Optical Properties ofE-4-(4-Dimethylaminostyryl)-1-methylpyridinium [DAMS⁺]. Journal of Physical Chemistry C, 2008, 112, 1213-1226.	1.5	20
76	The Role of Substituents on Functionalized 1,10-Phenanthroline in Controlling the Emission Properties of Cationic Iridium(III) Complexes of Interest for Electroluminescent Devices. Inorganic Chemistry, 2007, 46, 8533-8547.	1.9	164
77	Cyclometallated iridium(iii) complexes with substituted 1,10-phenanthrolines: a new class of highly active organometallic second order NLO-phores with excellent transparency with respect to second harmonic emission. Chemical Communications, 2007, , 4116.	2.2	87
78	Influence of the Sensitizer Adsorption Mode on the Open-Circuit Potential of Dye-Sensitized Solar Cells. Nano Letters, 2007, 7, 3189-3195.	4.5	340
79	Time-Dependent Density Functional Theory Investigations on the Excited States of Ru(II)-Dye-Sensitized TiO₂ Nanoparticles:â€‰ The Role of Sensitizer Protonation. Journal of the American Chemical Society, 2007, 129, 14156-14157.	6.6	228
80	Controlling Phosphorescence Color and Quantum Yields in Cationic Iridium Complexes:Â A Combined Experimental and Theoretical Study. Inorganic Chemistry, 2007, 46, 5989-6001.	1.9	237
81	Time-dependent and coupled-perturbed DFT and HF investigations on the absorption spectrum and non-linear optical properties of pushâ€“pull M(II)â€“porphyrin complexes (M=Zn, Cu, Ni). Chemical Physics Letters, 2007, 447, 10-15.	1.2	34
82	A high molar extinction coefficient charge transfer sensitizer and its application in dye-sensitized solar cell. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 185, 331-337.	2.0	159
83	An integrated computational tool for the study of the optical properties of nanoscale devices: application to solar cells and molecular wires. Theoretical Chemistry Accounts, 2007, 117, 1093-1104.	0.5	36
84	Efficient Green-Blue-Light-Emitting Cationic Iridium Complex for Light-Emitting Electrochemical Cells. Inorganic Chemistry, 2006, 45, 9245-9250.	1.9	193
85	A time-dependent density functional theory investigation on the nature of the electronic transitions involved in the nonlinear optical response of [Ru(CF3CO2)3T] (T = 4â€²-(C6H4-p-NBu2)-2,2â€²:6â€²,2â€³-terpyridine). Dalton Transactions, 2006, , 852-859.	[illegible]	20
86	Electronic Transitions Involved in the Absorption Spectrum and Dual Luminescence of Tetranuclear Cubane [Cu4I4(pyridine)4] Cluster:Â a Density Functional Theory/Time-Dependent Density Functional Theory Investigation. Inorganic Chemistry, 2006, 45, 10576-10584.	1.9	218
87	Synthesis, Characterization, and DFT-TDDFT Computational Study of a Ruthenium Complex Containing a Functionalized Tetradentate Ligand. Inorganic Chemistry, 2006, 45, 4642-4653.	1.9	167
88	Molecular Engineering of Organic Sensitizers for Solar Cell Applications. Journal of the American Chemical Society, 2006, 128, 16701-16707.	6.6	760
89	Ab initio molecular dynamics simulations of organometallic reactivity. Coordination Chemistry Reviews, 2006, 250, 1497-1513.	9.5	27
90	Time dependent density functional theory study of the absorption spectrum of the [Ru(4,4â€²-COOâˆ’-2,2â€²-bpy)2(X)2]4âˆ’ (X=NCS, Cl) dyes in water solution. Chemical Physics Letters, 2005, 415, 115-120.	1.2	91

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91	Mechanism of the Initial Conformational Transition of a Photomodulable Peptide. Angewandte Chemie - International Edition, 2005, 44, 6077-6081.	7.2	13
92	Photophysical Properties of [Ru(phen)2(dppz)]2+Intercalated into DNA:Â An Integrated Carâ˜Parrinello and TDDFT Study. Journal of the American Chemical Society, 2005, 127, 14144-14145.	6.6	112
93	Intramolecular Coupling of Î·2-Iminoacyls on Zirconium Bis(aryloxides) and Calix[4]arenes:Â Revised Mechanism by DFT Calculations and Carâ˜Parrinello Molecular Dynamics Simulations. Organometallics, 2005, 24, 1867-1875.	1.1	10
94	Combined Experimental and DFT-TDDFT Computational Study of Photoelectrochemical Cell Ruthenium Sensitizers. Journal of the American Chemical Society, 2005, 127, 16835-16847.	6.6	2,645
95	Time-dependent density functional theory study of the absorption spectrum of [Ru(4,4â€²-COOH-2,2â€²-bpy)2(NCS)2] in water solution: influence of the pH. Chemical Physics Letters, 2004, 389, 204-208.	1.2	121
96	A TDDFT study of the ruthenium(II) polyazaaromatic complex [Ru(dppz)(phen)2]2+ in solution. Chemical Physics Letters, 2004, 396, 43-48.	1.2	84
97	A Combined Computational and Experimental Study of Polynuclear Ruâ˜TPPZ Complexes:Â Insight into the Electronic and Optical Properties of Coordination Polymers. Journal of the American Chemical Society, 2004, 126, 9715-9723.	6.6	78
98	CASPT2//CASSCF and TDDFT//CASSCF Mapping of the Excited State Isomerization Path of a Minimal Model of the Retinal Chromophore. Journal of Physical Chemistry A, 2004, 108, 1208-1213.	1.1	82
99	The migratory insertion of carbon monoxide and methyl isocyanide into zirconium?carbon and titanium?carbon bonds anchored to a calix[4]arene moiety: a dynamical density functional study. Theoretical Chemistry Accounts, 2003, 110, 196-204.	0.5	10
100	A theoretical approach to a chemical system convertible into a storage cell: carbon_carbon bonds functioning as electron donor and electron acceptor units. Journal of Molecular Catalysis A, 2003, 204-205, 787-792.	4.8	1
101	Absorption Spectrum and Solvatochromism of the [Ru(4,4â€˜-COOH-2,2â€˜-bpy)2(NCS)2] Molecular Dye by Time Dependent Density Functional Theory. Journal of the American Chemical Society, 2003, 125, 4381-4387.	6.6	299
102	A Dynamic Density Functional Study of the Stepwise Migratory Insertion of Isocyanides into Zirconiumâ˜Carbon Bonds Anchored to a Calix[4]arene Moiety. Organometallics, 2002, 21, 4090-4098.	1.1	7
103	A density functional study of ethylene rearrangements assisted by tungsten calix[4]arenes. Dalton Transactions RSC, 2001, , 1718-1725.	2.3	8
104	Dynamical Density Functional Study of the Multistep CO Insertion into Zirconiumâ˜Carbon Bonds Anchored to a Calix[4]arene Moiety. Organometallics, 2001, 20, 4031-4039.	1.1	12
105	Density Functional Study of Tetraphenolate and Calix[4]arene Complexes of Early Transition Metals. Inorganic Chemistry, 2001, 40, 1544-1549.	1.9	11
106	Why does {p-But-calix[4]-(OMe)2(O)2ZrCl2} distort away from C2v symmetry?. Chemical Physics Letters, 1999, 315, 145-149.	1.2	1
107	Inertness of the Arylâ˜F Bond toward Oxidative Addition to Osmium and Rhodium Complexes:â€‰ Thermodynamic or Kinetic Origin?. Journal of the American Chemical Society, 1998, 120, 12634-12640.	6.6	90
108	Theoretical study of the metathesis-like reaction between ditungsten hexaalkoxides and alkynesâ€Šâ€. Journal of the Chemical Society Dalton Transactions, 1997, , 3845-3852.	1.1	12

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109	Oligomerization of the PH3CuCâ‹®CCuPH3 Acetylide toward the Formation of (PH3CuC)n (n = 4, 6, 8) Metal Carbides:â€‰ A Theoretical Study Based on Density Functional Theory. Inorganic Chemistry, 1997, 36, 2018-2022.	1.9	4