Simona Fantacci

List of Publications by Citations

108 papers	9,855 citations	44 h-index	99 g-index
110 ext. papers	10,342 ext. citations	6.7 avg, IF	5.84 L-index

#	Paper	IF	Citations
108	Combined experimental and DFT-TDDFT computational study of photoelectrochemical cell ruthenium sensitizers. *Journal of the American Chemical Society*, **2005**, 127, 16835-47	16.4	2503
107	Molecular engineering of organic sensitizers for solar cell applications. *Journal of the American Chemical Society*, **2006**, 128, 16701-7	16.4	728
106	Influence of the sensitizer adsorption mode on the open-circuit potential of dye-sensitized solar cells. *Nano Letters*, **2007**, 7, 3189-95	11.5	325
105	Theoretical studies on anatase and less common TiO2 phases: bulk, surfaces, and nanomaterials. *Chemical Reviews*, **2014**, 114, 9708-53	68.1	310
104	Absorption spectrum and solvatochromism of the [Ru(4,4-COOH-2,2-bpy)2(NCS)2] molecular dye by time dependent density functional theory. *Journal of the American Chemical Society*, **2003**, 125, 4381-7	16.4	289
103	Alignment of the dye molecular levels with the TiO(2) band edges in dye-sensitized solar cells: a DFT-TDDFT study. *Nanotechnology*, **2008**, 19, 424002	3.4	230
102	Controlling phosphorescence color and quantum yields in cationic iridium complexes: a combined experimental and theoretical study. *Inorganic Chemistry*, **2007**, 46, 5989-6001	5.1	226
101	High open-circuit voltage solid-state dye-sensitized solar cells with organic dye. *Nano Letters*, **2009**, 9, 2487-92	11.5	220
100	Time-dependent density functional theory investigations on the excited states of Ru(II)-dye-sensitized TiO2 nanoparticles: the role of sensitizer protonation. *Journal of the American Chemical Society*, **2007**, 129, 14156-7	16.4	220
99	Synthesis, characterization, and DFT/TD-DFT calculations of highly phosphorescent blue light-emitting anionic iridium complexes. *Inorganic Chemistry*, **2008**, 47, 980-9	5.1	212
98	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	3.8	200
97	Electronic transitions involved in the absorption spectrum and dual luminescence of tetranuclear cubane [Cu4I4(pyridine)4] cluster: a density functional theory/time-dependent density functional theory investigation. *Inorganic Chemistry*, **2006**, 45, 10576-84	5.1	200
96	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	3.8	192
95	Efficient green-blue-light-emitting cationic iridium complex for light-emitting electrochemical cells. *Inorganic Chemistry*, **2006**, 45, 9245-50	5.1	183
94	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, 8533-47	5.1	160
93	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	4.7	150
92	Synthesis, characterization, and DFT-TDDFT computational study of a ruthenium complex containing a functionalized tetradentate ligand. *Inorganic Chemistry*, **2006**, 45, 4642-53	5.1	147

91	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	23.2	143
90	Organic dyes incorporating low-band-gap chromophores based on extended benzothiadiazole for dye-sensitized solar cells. *Dyes and Pigments*, **2011**, 91, 192-198	4.6	142
89	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, 13538-48	16.4	131
88	Time-dependent density functional theory study of the absorption spectrum of [Ru(4,4?-COOH-2,2?-bpy)2(NCS)2] in water solution: influence of the pH. *Chemical Physics Letters*, **2004**, 389, 204-208	2.5	118
87	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	3.8	117
86	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	3.8	117
85	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	3.8	115
84	Photophysical properties of [Ru(phen)2(dppz)]2+ intercalated into DNA: an integrated Car-Parrinello and TDDFT study. *Journal of the American Chemical Society*, **2005**, 127, 14144-5	16.4	109
83	Electron-rich heteroaromatic conjugated bipyridine based ruthenium sensitizer for efficient dye-sensitized solar cells. *Chemical Communications*, **2008**, 5318-20	5.8	101
82	Simulating Dye-Sensitized TiO2 Heterointerfaces in Explicit Solvent: Absorption Spectra, Energy Levels, and Dye Desorption. *Journal of Physical Chemistry Letters*, **2011**, 2, 813-817	6.4	92
81	Cyclometalated iridium(III) complexes based on phenyl-imidazole ligand. *Inorganic Chemistry*, **2011**, 50, 451-62	5.1	87
80	Time dependent density functional theory study of the absorption spectrum of the [Ru(4,4?-COO2,2?-bpy)2(X)2]4 (X = NCS, Cl) dyes in water solution. *Chemical Physics Letters*, **2005**, 415, 115-120	2.5	86
79	White-light phosphorescence emission from a single molecule: application to OLED. *Chemical Communications*, **2009**, 4672-4	5.8	85
78	Inertness of the Aryl Bond toward Oxidative Addition to Osmium and Rhodium Complexes: Thermodynamic or Kinetic Origin?. *Journal of the American Chemical Society*, **1998**, 120, 12634-12640	16.4	83
77	A TDDFT study of the ruthenium(II) polyazaaromatic complex [Ru(dppz)(phen)2]2+ in solution. *Chemical Physics Letters*, **2004**, 396, 43-48	2.5	81
76	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**, 4116-8	5.8	79
75	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	2.8	79
74	A combined computational and experimental study of polynuclear Ru-TPPZ complexes: insight into the electronic and optical properties of coordination polymers. *Journal of the American Chemical Society*, **2004**, 126, 9715-23	16.4	78

73	Absorption and emission of the apigenin and luteolin flavonoids: a TDDFT investigation. *Journal of Physical Chemistry A*, **2009**, 113, 15118-26	2.8	70
72	Cyclometalated Ir(III) complexes with substituted 1,10-phenanthrolines: a new class of efficient cationic organometallic second-order NLO chromophores. *Chemistry - A European Journal*, **2010**, 16, 4814-25	5.8	60
71	Influence of Donor Groups of Organic D-A Dyes on Open-Circuit Voltage in Solid-State Dye-Sensitized Solar Cells. *Journal of Physical Chemistry C*, **2012**, 116, 1572-1578	3.8	59
70	Luminescent cyclometallated Ir(III) and Pt(II) complexes with beta-diketonate ligands as highly active second-order NLO chromophores. *Chemical Communications*, **2010**, 46, 2414-6	5.8	56
69	Panchromatic ruthenium sensitizer based on electron-rich heteroarylvinylene-conjugated quaterpyridine for dye-sensitized solar cells. *Dalton Transactions*, **2011**, 40, 234-42	4.3	52
68	Theoretical and experimental investigation on the spectroscopic properties of indigo dye. *Journal of Molecular Structure*, **2011**, 993, 43-51	3.4	52
67	Panchromatic cross-substituted squaraines for dye-sensitized solar cell applications. *ChemSusChem*, **2009**, 2, 621-4	8.3	49
66	From Blue to Green: Fine-Tuning of Photoluminescence and Electrochemiluminescence in Bifunctional Organic Dyes. *Journal of the American Chemical Society*, **2017**, 139, 2060-2069	16.4	48
65	Computational chemistry meets cultural heritage: challenges and perspectives. *Accounts of Chemical Research*, **2010**, 43, 802-13	24.3	45
64	Tuning the dipolar second-order nonlinear optical properties of cyclometalated platinum(II) complexes with tridentate N^C^N binding ligands. *Chemistry - A European Journal*, **2013**, 19, 9875-83	4.8	41
63	Time-Dependent Density Functional Theory Modeling of Spin-Orbit Coupling in Ruthenium and Osmium Solar Cell Sensitizers. *Journal of Physical Chemistry C*, **2014**, 118, 17067-17078	3.8	40
62	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	2.7	39
61	Complexation of apigenin and luteolin in weld lake: a DFT/TDDFT investigation. *Physical Chemistry Chemical Physics*, **2010**, 12, 6672-84	3.6	34
60	An inconvenient influence of iridium(III) isomer on OLED efficiency. *Dalton Transactions*, **2010**, 39, 8914-8	4.3	34
59	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	1.9	34
58	DFT/TDDFT investigation on the UV-vis absorption and fluorescence properties of alizarin dye. *Physical Chemistry Chemical Physics*, **2015**, 17, 6374-82	3.6	33
57	Time-dependent and coupled-perturbed DFT and HF investigations on the absorption spectrum and non-linear optical properties of push-pull M(II)-porphyrin complexes (M=Zn, Cu, Ni). *Chemical Physics Letters*, **2007**, 447, 10-15	2.5	32
56	Towards efficient sustainable full-copper dye-sensitized solar cells. *Dalton Transactions*, **2019**, 48, 9703-9711	4.3	31

55	Spectroscopic properties of cyclometallated iridium complexes by TDDFT. *Computational and Theoretical Chemistry*, **2009**, 914, 74-86		30
54	Photochemistry of Artists' Dyes and Pigments: Towards Better Understanding and Prevention of Colour Change in Works of Art. *Angewandte Chemie - International Edition*, **2018**, 57, 7324-7334	16.4	29
53	A Joint Experimental and Theoretical Investigation on Nonlinear Optical (NLO) Properties of a New Class of Push–Pull Spirobifluorene Compounds. *European Journal of Organic Chemistry*, **2010**, 2010, 4004-4016	3.2	28
52	Impact of Spin-Orbit Coupling on Photocurrent Generation in Ruthenium Dye-Sensitized Solar Cells. *Journal of Physical Chemistry Letters*, **2014**, 5, 375-80	6.4	27
51	A simple synthetic route to obtain pure trans-ruthenium(II) complexes for dye-sensitized solar cell applications. *ChemSusChem*, **2013**, 6, 2170-80	8.3	24
50	Ab initio molecular dynamics simulations of organometallic reactivity. *Coordination Chemistry Reviews*, **2006**, 250, 1497-1513	23.2	24
49	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, 252-60	3.6	23
48	Role of hot singlet excited states in charge generation at the black dye/TiO2 interface. *ACS Applied Materials & Interfaces*, **2013**, 5, 4334-9	9.5	23
47	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	3.8	22
46	An EFISH, Theoretical, and PGSE NMR Investigation on the Relevant Role of Aggregation on the Second Order Response in CHCl3 of the Push–Pull Chromophores [5-[[4?-(Dimethylamino)phenyl]ethynyl]-15-[(4??-nitrophenyl)ethynyl]-10,20-diphenylporphyrinate] M(II) (M = Zn, Ni). *Journal of Physical Chemistry C*, **2009**, 113, 11131-11141	3.8	20
45	Theoretical Investigations of the Effects of J-Aggregation on the Linear and Nonlinear Optical Properties of E-4-(4-Dimethylaminostyryl)-1-methylpyridinium [DAMS+]. *Journal of Physical Chemistry C*, **2008**, 112, 1213-1226	3.8	20
44	Designing Squaraines to Control Charge Injection and Recombination Processes in NiO-based Dye-Sensitized Solar Cells. *ChemSusChem*, **2017**, 10, 2385-2393	8.3	18
43	Everything you always wanted to know about black dye (but were afraid to ask): a DFT/TDDFT investigation. *Chimia*, **2013**, 67, 121-8	1.3	18
42	Computational Investigations on Organic Sensitizers for Dye-Sensitized Solar Cell. *Current Organic Synthesis*, **2012**, 9, 215-232	1.9	18
41	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 = 4N(C6H4-p-NBu2)-2,2N6,2N-terpyridine). *Dalton Transactions*, **2006**, 852-9	4.3	18
40	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	3.8	18
39	Cobalt Polypyridyl Complexes as Transparent Solution-Processable Solid-State Charge Transport Materials. *Advanced Energy Materials*, **2016**, 6, 1600874	21.8	17
38	Discoloration of the smalt pigment: experimental studies and ab initio calculations. *Journal of Analytical Atomic Spectrometry*, **2012**, 27, 1941	3.7	17

37	An investigation on the second order nonlinear optical response of tris-cyclometallated Ir(III) complexes with variously substituted 2-phenylpyridines. *Dalton Transactions*, **2013**, 42, 155-9	4.3	17
36	Structural and electronic properties of the PbCrO4 chrome yellow pigment and of its light sensitive sulfate-substituted compounds. *RSC Advances*, **2016**, 6, 36336-36344	3.7	17
35	Electronic and optical properties of dye-sensitized TiO□ interfaces. *Topics in Current Chemistry*, **2014**, 347, 1-45		16
34	New [(D-terpyridine)-Ru-(D or A-terpyridine)][4-EtPhCO2]2 complexes (D = electron donor group; A = electron acceptor group) as active second-order non linear optical chromophores. *Dalton Transactions*, **2012**, 41, 6707-14	4.3	16
33	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	2.1	16
32	Theoretical investigation of the structural and electronic properties of luteolin, apigenin and their deprotonated species. *Computational and Theoretical Chemistry*, **2008**, 868, 12-21		14
31	DFT/TDDFT investigation of the stepwise deprotonation in tetracycline: pKa assignment and UV□is spectroscopy. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	13
30	Mechanism of the initial conformational transition of a photomodulable peptide. *Angewandte Chemie - International Edition*, **2005**, 44, 6077-81	16.4	13
29	First member of an appealing class of cyclometalated 1,3-di-(2-pyridyl)benzene platinum(II) complexes for solution-processable OLEDs. *Journal of Materials Chemistry C*, **2020**, 8, 7873-7881	7.1	12
28	pH-Sensitive Bis(2,2?:6?,2"-terpyridine)ruthenium(II) Complexes □A DFT/TDDFT Investigation of Their Spectroscopic Properties. *European Journal of Inorganic Chemistry*, **2011**, 2011, 1605-1613	2.3	12
27	Acid□base chemistry of luteolin and its methyl-ether derivatives: A DFT and ab initio investigation. *Chemical Physics Letters*, **2008**, 462, 313-317	2.5	12
26	Dynamical Density Functional Study of the Multistep CO Insertion into Zirconium□carbon Bonds Anchored to a Calix[4]arene Moiety. *Organometallics*, **2001**, 20, 4031-4039	3.8	12
25	Tuning the dipolar second-order nonlinear optical properties of 5-□delocalized-donor-1,3-di(2-pyridyl)benzenes, related cyclometallated platinum(ii) complexes and methylated salts. *Dalton Transactions*, **2017**, 46, 1179-1185	4.3	10
24	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		10
23	Density functional study of tetraphenolate and calix[4]arene complexes of early transition metals. *Inorganic Chemistry*, **2001**, 40, 1544-9	5.1	10
22	A Chiral Bis(salicylaldiminato)zinc(II) Complex with Second-Order Nonlinear Optical and Luminescent Properties in Solution. *Inorganics*, **2020**, 8, 25	2.9	9
21	Theoretical study of the metathesis-like reaction between ditungsten hexaalkoxides and alkynes□ *Journal of the Chemical Society Dalton Transactions*, **1997**, 3845-3852		9
20	Intramolecular Coupling of □-Iminoacyls on Zirconium Bis(aryloxides) and Calix[4]arenes: Revised Mechanism by DFT Calculations and Car□Parrinello Molecular Dynamics Simulations. *Organometallics*, **2005**, 24, 1867-1875	3.8	9

19	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	1.9	9
18	Design of cyclometallated 5-□delocalized donor-1,3-di(2-pyridyl)benzene platinum(II) complexes with second-order nonlinear optical properties. *Polyhedron*, **2018**, 140, 74-77	2.7	9
17	Novel cyclometallated 5-□delocalized donor-1,3-di(2-pyridyl)benzene platinum(ii) complexes with good second-order nonlinear optical properties. *Dalton Transactions*, **2018**, 48, 202-208	4.3	8
16	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, 8374-6	5.8	8
15	A density functional study of ethylene rearrangements assisted by tungsten calix[4]arenes. *Dalton Transactions RSC*, **2001**, 1718-1725		8
14	Design of Ru(II) sensitizers endowed by three anchoring units for adsorption mode and light harvesting optimization. *Thin Solid Films*, **2014**, 560, 86-93	2.2	7
13	A Dynamic Density Functional Study of the Stepwise Migratory Insertion of Isocyanides into Zirconium□Carbon Bonds Anchored to a Calix[4]arene Moiety. *Organometallics*, **2002**, 21, 4090-4098	3.8	6
12	Ab Initio Modeling of Solar Cell Dye Sensitizers: The Hunt for Red Photons Continues. *European Journal of Inorganic Chemistry*, **2019**, 2019, 743-750	2.3	5
11	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	3.8	5
10	Perylenetetracarboxy-3,4:9,10-diimide derivatives with large two-photon absorption activity. *New Journal of Chemistry*, **2019**, 43, 1885-1893	3.6	4
9	A combined theoretical and experimental investigation of the electronic and vibrational properties of red lead pigment. *Journal of Cultural Heritage*, **2020**, 46, 374-381	2.9	4
8	Oligomerization of the PH(3)CuC&tbd1;CCuPH(3) Acetylide toward the Formation of (PH(3)CuC)(n)() (n = 4, 6, 8) Metal Carbides: A Theoretical Study Based on Density Functional Theory. *Inorganic Chemistry*, **1997**, 36, 2018-2022	5.1	4
7	A computational approach to the electronic, optical and acid□base properties of Ru(II) dyes for photoelectrochemical solar cells applications. *Polyhedron*, **2014**, 82, 88-103	2.7	2
6	Theoretical Study of the Structural and Electronic Properties of Luteolin and Apigenin Dyes. *Lecture Notes in Computer Science*, **2008**, 1141-1155	0.9	2
5	Mechanism of the Initial Conformational Transition of a Photomodulable Peptide. *Angewandte Chemie*, **2005**, 117, 6231-6235	3.6	2
4	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	4.7	2
3	Why does {p-But-calix[4]-(OMe)2(O)2ZrCl2} distort away from C2v symmetry?. *Chemical Physics Letters*, **1999**, 315, 145-149	2.5	1
2	Zur Photochemie von K□nstlerfarben: Strategien zur Verhinderung von Farbver□derungen in Kunstwerken. *Angewandte Chemie*, **2018**, 130, 7447-7457	3.6	1

1	Modelling the Interaction between Carboxylic Acids and Zinc Oxide: Insight into Degradation of ZnO Pigments. *Molecules*, **2022**, 27, 3362	4.8	0