Francesco Lelj

List of Publications by Year
in descending order

62 papers	1,804 citations	279798 23 h-index	276875 41 g-index
62 all docs	62 docs citations	62 times ranked	2315 citing authors

#	Article	IF	Citations
1	Halogen bonding in metalâ€“organicâ€“supramolecular networks. Coordination Chemistry Reviews, 2010, 254, 677-695.	18.8	332
2	New [M(R,Râ€˜timdt)2] Metal-Dithiolenes and Related Compounds (M = Ni, Pd, Pt; R,Râ€˜timdt = Monoanion) Tj ETQq0 0 0 rgBT /Overlo of the American Chemical Society, 1999, 121, 7098-7107.	13.7	85
3	Discotic mesomorphism of 2,3,7,8,12,13,17,18-octakis (alkyl-thio) 5,10,15,20 tetraaza porphyrin and its complexes with some divalent transition metal ions Synthesis and characterization. Liquid Crystals, 1992, 12, 941-960.	2.2	83
4	Halogen Bond in (CH3)nX (X = N, P,n= 3; X = S,n= 2) and (CH3)nXO (X = N, P,n= 3; X = S,n= 2) Adducts with CF3I. Structural and Energy Analysis Including Relativistic Zero-Order Regular Approximation Approach in a Density Functional Theory Framework. Journal of Physical Chemistry A, 2002, 106, 9114-9119.	2.5	77
5	Capsule Formation, Carboxylate Exchange, and DFT Exploration of Cadmium Cluster Metallocavitands: Highly Dynamic Supramolecules. Journal of the American Chemical Society, 2010, 132, 3893-3908.	13.7	75
6	Mechanistic Aspects of the Reaction between Br2 and Chalcogenone Donors (LE; E=S, Se): Competitive Formation of 10-E-3, T-Shaped 1:1 Molecular Adducts, Charge-Transfer Adducts, and [(LE)2]2+ Dications. Chemistry - A European Journal, 2001, 7, 3122-3133.	3.3	68
7	Luminescent Compounds fac- and mer-Aluminum Tris(quinolin-8-olate). A Pure and Hybrid Density Functional Theory and Time-Dependent Density Functional Theory Investigation of Their Electronic and Spectroscopic Properties. Journal of Physical Chemistry A, 2003, 107, 2560-2569.	2.5	67
8	Spectroscopy and electrochemical properties of a homologous series of acetylacetonato and hexafluoroacetylacetonato cyclopalladated and cycloplatinated complexes. Dalton Transactions, 2008, , 4303.	3.3	57
9	Optical non-linear properties of the [MXY] neutral mixed-ligand dithiolenes (M=Ni, Pd, Pt; X=R2timdt,) Tj ETQq1 1 0.784314 rgBT /Ov excited states. Chemical Physics Letters, 2003, 372, 51-58.	2.6	47
10	Absorption Spectra of the Potential Photodynamic Therapy Photosensitizers Texaphyrins Complexes:â€‰ A Theoretical Analysis. Journal of Chemical Theory and Computation, 2007, 3, 860-869.	5.3	38
11	Investigations on the electronic effects of the peripheral 4â€²-group on 5-(4â€²-substituted)phenylazo-8-hydroxyquinoline ligands: zinc and aluminium complexes. Dalton Transactions, 2004, , 2424-2431.	3.3	36
12	Tuning the Emission Lifetime in Bis-cyclometalated Iridium(III) Complexes Bearing Iminopyrene Ligands. Inorganic Chemistry, 2014, 53, 11882-11889.	4.0	34
13	Inter-ring interactions and peripheral tail effects on the discotic mesomorphism of â€˜free-baseâ€™ and Co(ii), Ni(ii) and Cu(ii) alkenyl(sulfanyl) porphyrazines. Journal of Materials Chemistry, 2000, 10, 297-304.	6.7	33
14	Linkage Isomerism in Silver Acylpyrazolonato Complexes and Correlation with Their Antibacterial Activity. Inorganic Chemistry, 2016, 55, 5453-5466.	4.0	33
15	Synthesis, X-ray crystal structure and spectroscopic characterization of the new dithiolene [Pd(Et2timdt)2] and of its adduct with molecular diiodine [Pd(Et2timdt)2]Â·I2Â·CHCl3 (Et2timdtâ€…=â€…monoanion of 1,3-diethylimidazolidine-2,4,5-trithione). Journal of the Chemical Society Dalton Transactions, 1998, , 3731-3736.	1.1	32
16	8-Hydroxyquinoline Monomer, Water Adducts, and Dimer. Environmental Influences on Structure, Spectroscopic Properties, and Relative Stability of Cis and Trans Conformers. Journal of Physical Chemistry A, 2007, 111, 13403-13414.	2.5	32
17	Liaisons between photoconductivity and molecular frame in organometallic Pd(ii) and Pt(ii) complexes. Journal of Materials Chemistry, 2011, 21, 13434.	6.7	27
18	Elucidating the Origin of Enhanced Phosphorescence Emission in the Solid State (EPESS) in Cyclometallated Iridium Complexes. European Journal of Inorganic Chemistry, 2014, 2014, 3657-3664.	2.0	27

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19	Monolayers and Langmuir-Blodgett Films of a Newly Synthesized Asymmetric Tetraazaporphyrin Derivative. The Journal of Physical Chemistry, 1994, 98, 10613-10620.	2.9	26
20	Synthesis, structure, magnetic, spectroscopic and electrochemical behaviour of chloro-iron(III) and -manganese(III) complexes of 2,3,7,8,12,13,17,18-octakis(ethylsulfanyl)-5,10,15,20-tetraazaporphyrin. Journal of the Chemical Society Dalton Transactions, 1996, , 2799.	1.1	25
21	Organometallic red-emitting chromophores: a computational and experimental study on cyclometallated Nile Red complexes of palladium(ii) and platinum(ii) acetylacetonates and hexafluoroacetylacetonates. Dalton Transactions, 2008, , 6563.	3.3	25
22	Regioselectivity in the Nitration of Dialkoxybenzenes. Journal of Organic Chemistry, 2011, 76, 1285-1294.	3.2	24
23	Mono- and multilayer films of discotic metal-(alkythio)tetraazaporphyrins. The Journal of Physical Chemistry, 1993, 97, 9181-9186.	2.9	23
24	Inducing asymmetry in free-base, MnIII, NiII and CuII (ethylsulfanyl)porphyrazines: synthetic aspects and spectro-electrochemical implications. Dalton Transactions RSC, 2001, , 1143-1150.	2.3	22
25	Limits in the second-order response of [M(H2imXdt) (H2imYdt)] neutral complexes (M=Ni, Pd, Pt;) Tj ETQq1 1 0.784314 rgBT /Overlo theoretical study based on TD-DFT approach and ZORA formalism. Computational and Theoretical Chemistry, 2003, 636, 23-37.	1.5	22
26	Role of Entropy and Autosolvation in Dimerization and Complexation of C₆₀ by Zn₇ Metallocavitands. Inorganic Chemistry, 2012, 51, 3443-3453.	4.0	22
27	Pyridine imines as ligands in luminescent iridium complexes. Dalton Transactions, 2014, 43, 4026-4039.	3.3	22
28	Thioethylâ€Porphyrazine/Nanocarbon Hybrids for Photoinduced Electron Transfer. Advanced Functional Materials, 2018, 28, 1705418.	14.9	22
29	The Rich Tautomeric Behavior of Campestarenes. Chemistry - A European Journal, 2016, 22, 17657-17672.	3.3	20
30	Role of methyl substitution on the spectroscopic properties of porphyrazines. A TDDFT study using pure and hybrid functionals on porphyrazine and its octamethyl derivative. Chemical Physics Letters, 2003, 367, 308-318.	2.6	19
31	Blue emitting pentacoordinated Al(iii) complexes based on 2-methylquinolin-8-olate and substituted phenolate ligands. The role of phenolate derivatives on emission and absorption properties. Dalton Transactions, 2006, , 330-339.	3.3	19
32	Kinetic and Thermodynamic Aspects of the CT and T-Shaped Adduct Formation Between 1,3-Dimethylimidazoline-2-thione (or -2-selone) and Halogens. European Journal of Inorganic Chemistry, 2006, 2006, 2166-2174.	2.0	19
33	Atomistic simulation of discotic liquid crystals: Transition from isotropic to columnar phase example. Journal of Chemical Physics, 2007, 127, 134506.	3.0	19
34	Non-symmetrical aryl- and arylethynyl-substituted thioalkyl-porphyrazines for optoelectronic materials: synthesis, properties, and computational studies. Dalton Transactions, 2015, 44, 2191-2207.	3.3	19
35	Synthesis, Spectroscopy and Electrochemistry of Lanthanide Bis-(ethylsulfanyl)tetraazaporphyrins. Journal of Porphyrins and Phthalocyanines, 1998, 02, 177-188.	0.8	18
36	Synthesis of Heteroaryl Imines:Â Theoretical and Experimental Approach to the Determination of the Configuration of CN Double Bond. Journal of Organic Chemistry, 2006, 71, 7165-7179.	3.2	18

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37	Monolayers and Langmuir-Blodgett films of a new lutetium(III)-bis-octakis(alkylthio)tetraazaporphyrin. Thin Solid Films, 1994, 243, 310-315.	1.8	17
38	Cyclometalated Pt(iv) trans-diiodo adducts: experimental and computational studies within an homologous series of compounds. Dalton Transactions, 2011, 40, 5259.	3.3	17
39	Stereochemical Stability and Absolute Configuration of Atropisomeric Alkylthioporphyrazines by Dynamic NMR and HPLC Studies and Computational Analysis of HPLCâ€ECD Recorded Spectra. European Journal of Organic Chemistry, 2018, 2018, 4029-4037.	2.4	17
40	Deuteration of Aromatic Rings under Very Mild Conditions through Keto-Enamine Tautomeric Amplification. Journal of Organic Chemistry, 2015, 80, 5144-5150.	3.2	16
41	Two-electron reduction of alkyl(sulfanyl)porphyrazines: a route to free-base and peripherally metallated asymmetric porphyrazines. Dalton Transactions, 2004, , 305-312.	3.3	15
42	Effect of polyfluorination on self-assembling and electronic properties of thioalkyl-porphyrazines. Journal of Porphyrins and Phthalocyanines, 2016, 20, 223-233.	0.8	15
43	Crystal structure of high-spin (S= 5/2) manganese(II) 2,3,7,8,12,13,17,18-octakis(ethylsulfanyl)-5,10,15,20-tetraazaporphyrinate. Journal of the Chemical Society Dalton Transactions, 1996, , 3243.	1.1	13
44	Experimental and computational evidence of the intermolecular motifs in the crystal packing of luminescent pentacoordinated gallium(iii) complexes. Dalton Transactions, 2006, , 5124.	3.3	13
45	Atropisomerism in a thermally switchable, cyclometallated iridium complex. Dalton Transactions, 2012, 41, 10150.	3.3	11
46	Competition between Bailar and Ray-Dutt paths in conformational interconversion of tris-chelated complexes: a DFT study. Theoretical Chemistry Accounts, 2008, 120, 447-457.	1.4	10
47	Columnar Discotic Mesophases from Novel Non-symmetrically Substituted (Octylsulfanyl) Porphyrazines. Molecular Crystals and Liquid Crystals, 2008, 481, 56-72.	0.9	10
48	Expanded campestarene hosts for tetra- and dinuclear uranyl(<scp>vi</scp>) complexes. Chemical Communications, 2018, 54, 11869-11872.	4.1	10
49	New Investigations of Geometric, Electronic, and Spectroscopic Properties of Tetrapyrrolic Macrocycles by a TDâ^'DFT Approach. Carbon, Nitrogen, and Chalcogen (O, S, Se) Peripheral Substitution Effects on Ni(II) Porphyrazinato Complexes. Journal of Chemical Theory and Computation, 2007, 3, 833-851.	5.3	9
50	Structural and new spectroscopic properties of neutral $$[hbox{M(dmit)}_{f 2}] (hbox{dmit} =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 2 $$[hbox{M}(hbox{H}_{f 2}hbox{timdt})_{f 2}](hbox{H}_{f 2}hbox{timdt} = hbox{H}_{f 2}) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 222 Chemistry Accounts, 2007, 117, 621-635.	1.4	9
51	Bis(cyclopentadienyl)dihydrido Mo and W complexes as Lewis bases â€" A computational study about their adducts with BX₃(X = F, Cl) and Al(CH₃)₃. Canadian Journal of Chemistry, 2009, 87, 1406-1414.	1.1	9
52	Programming permanent and transient molecular protection via mechanical stoppering. Chemical Science, 2019, 10, 10422-10427.	7.4	8
53	Emissive Ir(iii) complexes bearing thienylamido groups on a 1,10-phenanthroline scaffold. Dalton Transactions, 2015, 44, 16272-16279.	3.3	7
54	Ground and Excited States of [M(H2timdt)2] Neutral Dithiolenes (M = Ni, Pd, Pt; H2timdt = Monoanion) Tj ETQq0 0 0 rgBT /Overlock 10 Journal of Physical Chemistry A, 2003, 107, 9679-9687.	2.5	6

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55	Trans influence and substituent effects on the HOMO-LUMO energy gap and Stokes shift in Ru mono-diimine derivatives. Journal of Molecular Structure, 2019, 1195, 620-631.	3.6	6
56	Tandem Photoarylationâ€“Photoisomerization of Halothiazoles: Synthesis, Photophysical and Singlet Oxygen Activation Properties of Ethyl 2â€Arylthiazoleâ€5â€carboxylates. European Journal of Organic Chemistry, 2010, 2010, 3416-3427.	2.4	5
57	Fluorine Interactions in the 3D Packing of â€œPt(IV)I₂â€•Organometallic Molecular Materials: Structural and Computational Approaches. Crystal Growth and Design, 2017, 17, 409-413.	3.0	4
58	Diverse binding of cationic guests by highly substituted [3 + 3] Schiff-base macrocycles. Organic Chemistry Frontiers, 2021, 8, 1437-1446.	4.5	4
59	Effects of methyl groups in a pyrimidine-based flexible ligand on the formation of silver(<scp>i</scp>) coordination networks. New Journal of Chemistry, 2018, 42, 13998-14008.	2.8	3
60	Photoconductive Properties and Electronic Structure in 3,5-Disubstituted 2-(2â€²-Pyridyl)Pyrroles Coordinated to a Pd(II) Salicylideneiminate Synthon. Inorganic Chemistry, 2021, 60, 9287-9301.	4.0	2
61	Breathing Room: Restoring Free Rotation in a Schiff-Base Macrocycle through Endoperoxide Formation. Organic Letters, 2021, 23, 9538-9542.	4.6	1
62	An Interplay Between Infrared Multiphoton Dissociation Fourier-Transform Ion Cyclotron Resonance Mass Spectrometry and Density Functional Theory Computations in the Characterization of a Tripodal Quinolin-8-Olate Gd(III) Complex. Journal of the American Society for Mass Spectrometry, 2013, 24, 589-601.	2.8	0