Silvia Carlotto

List of Publications by Year
in descending order

64	732	516561 16	642610 23
papers	citations	h-index	g-index

66	66	66	827
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Unraveling Solvent-Driven Equilibria between Î±- and 3₁₀-Helices through an Integrated Spin Labeling and Computational Approach. Journal of the American Chemical Society, 2007, 129, 11248-11258.	6.6	40
2	Dimers of polar chromophores in solution: role of excitonic interactions in one- and two-photon absorption properties. Physical Chemistry Chemical Physics, 2011, 13, 11099.	1.3	39
3	Ab InitioModeling of CW-ESR Spectra of the Double Spin Labeled Peptide Fmoc-(Aib-Aib-TOAC)2-Aib-OMe in Acetonitrile. Journal of Physical Chemistry B, 2007, 111, 2668-2674.	1.2	32
4	Energetics of CO oxidation on lanthanide-free perovskite systems: the case of Co-doped SrTiO₃. Physical Chemistry Chemical Physics, 2016, 18, 33282-33286.	1.3	29
5	Catalytic Mechanisms of NO Reduction in a COâ€“NO Atmosphere at Co- and Cu-Doped SrTiO₃(100) Surfaces. Journal of Physical Chemistry C, 2018, 122, 449-454.	1.5	28
6	Co- and Cu-Doped Titanates: Toward a New Generation of Catalytic Converters. Catalysis Letters, 2014, 144, 1466-1471.	1.4	27
7	Adaptive helicity and chiral recognition in bright europium quadruple-stranded helicates induced by host-guest interaction. Cell Reports Physical Science, 2022, 3, 100692.	2.8	27
8	Multipolar symmetric squaraines with large two-photon absorption cross-sections in the NIR region. Physical Chemistry Chemical Physics, 2011, 13, 12087.	1.3	26
9	Adsorption of small molecules at the cobalt-doped SrTiO3(001) surface: A first-principles investigation. Surface Science, 2015, 633, 68-76.	0.8	25
10	Electronic structure of SrTi1â^'xMxO3â^'Î´ (M=Co, Ni, Cu) perovskite-type doped-titanate crystals by DFT and DFT+U calculations. Chemical Physics Letters, 2013, 588, 102-108.	1.2	24
11	The electronic properties of three popular high spin complexes [TM(acac)₃, TM = Cr, Mn, and Fe] revisited: an experimental and theoretical study. Physical Chemistry Chemical Physics, 2017, 19, 24840-24854.	1.3	22
12	Adsorption of CO and formation of carbonates at steps of pure and Co-doped SrTiO3 surfaces by DFT calculations. Applied Surface Science, 2016, 364, 522-527.	3.1	21
13	Electronic structure of CuTPP and CuTPP(F) complexes: a combined experimental and theoretical study II. Physical Chemistry Chemical Physics, 2016, 18, 24890-24904.	1.3	19
14	Reaction of Copper(II) Chloroacetate with Pyrazole. Synthesis of a One-Dimensional Coordination Polymer and Unexpected Dehydrochlorination Reaction. Crystal Growth and Design, 2015, 15, 5910-5918.	1.4	18
15	Theoretical modeling of the L_{2,3}-edge X-ray absorption spectra of Mn(acac)₂and Co(acac)₂complexes. Physical Chemistry Chemical Physics, 2016, 18, 2242-2249.	1.3	17
16	Electronic structures of CuTPP and CuTPP(F) complexes. A combined experimental and theoretical study I. Physical Chemistry Chemical Physics, 2016, 18, 18727-18738.	1.3	16
17	L_{2,3}-edges absorption spectra of a 2D complex system: a theoretical modelling. Physical Chemistry Chemical Physics, 2016, 18, 28110-28116.	1.3	16
18	Ferrous to Ferric Transition in Feâ€Phthalocyanine Driven by NO₂ Exposure. Chemistry - A European Journal, 2021, 27, 3526-3535.	1.7	16

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19	Integrated Approach for Modeling the Emission Fluorescence of 4-(N,N-Dimethylamino)benzonitrile in Polar Environments. Journal of Physical Chemistry B, 2008, 112, 8106-8113.	1.2	15
20	Mn(acac) 2 and Mn(acac) 3 complexes, a theoretical modeling of their L 2,3 -edges X-ray absorption spectra. Polyhedron, 2017, 135, 216-223.	1.0	14
21	Theoretical Investigation of the Electronic Properties of Three Vanadium Phthalocyaninato (Pc) Based Complexes: PcV, PcVO, and PcVI. Inorganic Chemistry, 2018, 57, 1859-1869.	1.9	13
22	Substrate involvement in dioxygen bond dissociation catalysed by iron phthalocyanine supported on Ag(100). Chemical Communications, 2018, 54, 9418-9421.	2.2	13
23	Coordinative unsaturated Cu^I entities are crucial intermediates governing cell internalization of copper. A combined experimental ESI-MS and DFT study. Metallomics, 2019, 11, 1800-1804.	1.0	12
24	Luminescent Thermometers: From a Library of Europium(III) Î²â€Diketonates to a General Model for Predicting the Thermometric Behaviour of Europiumâ€Based Coordination Systems. ChemPhotoChem, 2020, 4, 674-684.	1.5	12
25	The role of the dopant and structural defects on the water absorption and on the H2 formation in the Al, Co and Cu doped SrTiO3 perovskite steps. Applied Surface Science, 2020, 527, 146850.	3.1	12
26	On-surface synthesis of extended linear graphyne molecular wires by protecting the alkynyl group. Physical Chemistry Chemical Physics, 2020, 22, 12180-12186.	1.3	12
27	Computational Study of Environmental Effects on Torsional Free Energy Surface of N-Acetyl-Nâ€²-methyl-l-alanylamide Dipeptide. Journal of Chemical Education, 2014, 91, 96-102.	1.1	11
28	Comparative Experimental and Theoretical Study of the Fe L_{2,3}-Edges X-ray Absorption Spectroscopy in Three Highly Popular, Low-Spin Organoiron Complexes: [Fe(CO)₅], [(Î·⁵-C₅H₅)Fe(CO)(Î¼-CO)]₂, and [(Î·⁵-C₅H₅)₂Fe]. Inorganic Chemistry, 2019, 58, 5844-5857.	1.9	11
29	Multireference Ab Initio Investigation on Ground and Low-Lying Excited States: Systematic Evaluation of Jâ€“J Mixing in a Eu³⁺ Luminescent Complex. Inorganic Chemistry, 2021, 60, 315-324.	1.9	11
30	Time correlated fluorescence characterization of an asymmetrically focused flow in a microfluidic device. Microfluidics and Nanofluidics, 2011, 10, 551-561.	1.0	10
31	Reversible redox reactions in metal-supported porphyrin: the role of spin and oxidation state. Journal of Materials Chemistry C, 2021, 9, 12559-12565.	2.7	10
32	Charge Transfer in Model Bioinspired Caroteneâ€“Porphyrin Dyads. Journal of Physical Chemistry A, 2012, 116, 3926-3933.	1.1	9
33	â€œPigments of Lifeâ€: Molecules Well Suited to Investigate Metalâ€“Ligand Symmetryâ€Restricted Covalency. European Journal of Inorganic Chemistry, 2018, 2018, 3145-3155.	1.0	9
34	Theoretical Investigation of the Open Circuit Voltage: P3HT/9,9â€²-Bisfluorenylidene Derivative Devices. Journal of Physical Chemistry A, 2014, 118, 4808-4815.	1.1	7
35	New light on an old debate: does the RCNâ€“PtCl₂ bond include any back-donation? RCNâ†’PtCl₂ backbonding vs. the IR Î½_{Cî€,N} blue-shift dichotomy in organonitrilesâ€“platinum(ⁱⁱ) complexes. A thorough density functional theory â€“ energy decomposition analysis study. Dalton Transactions, 2019, 48, 12974-12985.	1.6	7
36	Comparative Experimental and Theoretical Study of the C and O K-Edge X-ray Absorption Spectroscopy in Three Highly Popular, Low Spin Organoiron Complexes: [Fe(CO)₅], [(Î·⁵-C₅H₅)Fe(CO)(Î¼-CO)]₂, and [(Î·⁵-C₅H₅)₂Fe]. Inorganic Chemistry, 2019, 58, 16411-16423.	1.9	7

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37	Antenna triplet DFT calculations to drive the design of luminescent Ln³⁺complexes. Dalton Transactions, 2020, 49, 14556-14563.	1.6	7
38	Small Copper Clusters Supported on SrTiO₃: An Experimental and Theoretical Study. European Journal of Inorganic Chemistry, 2018, 2018, 3829-3834.	1.0	6
39	Spin state, electronic structure and bonding on C-scorpionate [Fe(II)Cl2(tpm)] catalyst: An experimental and computational study. Catalysis Today, 2020, 358, 403-411.	2.2	6
40	Adsorption and reactivity of CO at a stepped SrTiO3(1Â0Â0) surface in the presence of Cu impurities. Applied Surface Science, 2020, 521, 146450.	3.1	6
41	Heterovalent BiIII/PbII Ionic Substitution in One-Dimensional Trimethylsulfoxonium Halide Pseudo-Perovskites (X = I, Br). Journal of Physical Chemistry C, 2021, 125, 11728-11742.	1.5	6
42	A Theoretical Study of the Occupied and Unoccupied Electronic Structure of High- and Intermediate-Spin Transition Metal Phthalocyaninato (Pc) Complexes: VPc, CrPc, MnPc, and FePc. Nanomaterials, 2021, 11, 54.	1.9	6
43	Bi3+ doping in 1D ((CH3)3SO)PbI3: a model for defect interactions in halide perovskites. Journal of Materials Chemistry C, 2022, 10, 1458-1469.	2.7	6
44	In Silico Interpretation of cw-ESR at 9 and 95 GHz of Mono- and bis- TOAC-Labeled Aib-Homopeptides in Fluid and Frozen Acetonitrile. Journal of Physical Chemistry B, 2011, 115, 13026-13036.	1.2	5
45	Distortion-driven spin switching in electron-doped metal porphyrins. Journal of Materials Chemistry C, 2022, 10, 9748-9757.	2.7	5
46	Evaluation of translational friction coefficients of macroscopic probes in nematic liquid crystals. Journal of Chemical Physics, 2008, 128, 154505.	1.2	4
47	Trinuclear Cu(II) complexes from the classic [Cu 2 (RCOO) 4 (H 2 O) 2] lantern complex and pyrazole: a DFT modelling of the reaction path. Inorganica Chimica Acta, 2018, 470, 93-99.	1.2	4
48	Mnâ€“Cu Transmetalation as a Strategy for the Assembly of Decoupled Metalâ€“Organic Networks on Sn/Cu(001) Surface Alloys. Journal of Physical Chemistry C, 2020, 124, 18993-19002.	1.5	4
49	Nature of the Ligand-Centered Triplet State in Gd3+ Î²-Diketonate Complexes as Revealed by Time-Resolved EPR Spectroscopy and DFT Calculations. Inorganic Chemistry, 2021, 60, 15141-15150.	1.9	4
50	The Magnetic Behaviour of CoTPP Supported on Coinage Metal Surfaces in the Presence of Small Molecules: A Molecular Cluster Study of the Surface trans-Effect. Nanomaterials, 2022, 12, 218.	1.9	4
51	An experimental and theoretical study of metallorganic coordination networks of tetrahydroxyquinone on Cu(111). New Journal of Chemistry, 2019, 43, 19186-19192.	1.4	3
52	Stabilization of high-spin Mn ions in tetra-pyrrolic configuration on copper. Applied Surface Science, 2021, 551, 149307.	3.1	3
53	An integrated approach for the interpretation of emission fluorescence of DMABN-Crown derivatives in polar environments. Chemical Physics Letters, 2008, 467, 204-209.	1.2	2
54	Heuristic approaches to the optimization of acceptor systems in bulk heterojunction cells: a computational study. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	2

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55	DFT modelling of the CO-NO redox reaction at Cu-doped SrTiO3(1Â0Â0) stepped surface: CO oxidation at lattice O ions. Inorganica Chimica Acta, 2020, 511, 119810.	1.2	2
56	A DFT mechanistic study of the synthesis of trans-Z,Z-[PtIICl(NH3){HNÂ=ÂC(NH2)Me}2]Cl from addition of NH3 to trans-[PtIICl2(N CMe)2]. Inorganica Chimica Acta, 2020, 511, 119847.	1.2	2
57	DFT modelling of the NO reduction process at the Cu-doped SrTiO3(1Â0Â0) stepped surface. Inorganica Chimica Acta, 2020, 511, 119813.	1.2	2
58	Interpretation of the emission fluorescence spectra of two fluoroionophores: DMABNâ€Crown4 and DMABNâ€Crown5. International Journal of Quantum Chemistry, 2010, 110, 368-375.	1.0	1
59	cis-[(Î·5-C5H5)Fe(Î·1-CO)(Î¼-CO)]2, the poor relative between cis and trans tautomers. A theoretical study of the gas-phase Fe L3-edge and C and O K-edge XAS of trans-/cis-[(Î·5-C5H5)Fe(Î·1-CO)(Î¼-CO)]2. Physical Chemistry Chemical Physics, 2021, 23, 24661-24668.	1.3	1
60	Evaluation of translational friction coefficients of micro-sized spherical probes in nematic liquid crystals. Theoretical Chemistry Accounts, 2008, 120, 591-597.	0.5	0
61	Time-Evolution Equations for Particle Dispersions in Nematic Liquid Crystal Media. Molecular Crystals and Liquid Crystals, 2010, 516, 167-173.	0.4	0
62	Luminescent Thermometers: From a Library of Europium(III) Î²â€Diketonates to a General Model for Predicting the Thermometric Behaviour of Europiumâ€Based Coordination Systems. ChemPhotoChem, 2020, 4, 646.	1.5	0
63	Strategy for the improvement of mixing in microdevices. Houille Blanche, 2011, 97, 79-85.	0.3	0
64	Donation and back-donation in cis- and trans-[(Î·5-C5H5)Fe(Î·1-CO)(Î¼-CO)]2 tautomers: Which relative is more generous? An ETS-NOCV bond analysis. Inorganica Chimica Acta, 2022, 536, 120897.	1.2	0