Maurizio Casarin

List of Publications by Year
in descending order

101	2,883	218592	189801
papers	citations	26 h-index	50 g-index

104	104	104	4025
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	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
3	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
4	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
5	On surface chemical reactions of free-base and titanyl porphyrins with r-TiO₂(110): a unified picture. Physical Chemistry Chemical Physics, 2022, 24, 12719-12744.	1.3	4
6	Distortion-driven spin switching in electron-doped metal porphyrins. Journal of Materials Chemistry C, 2022, 10, 9748-9757.	2.7	5
7	Ferrous to Ferric Transition in Feâ€Phthalocyanine Driven by NO₂ Exposure. Chemistry - A European Journal, 2021, 27, 3526-3535.	1.7	16
8	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
9	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
10	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
11	Stabilization of high-spin Mn ions in tetra-pyrrolic configuration on copper. Applied Surface Science, 2021, 551, 149307.	3.1	3
12	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
13	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
14	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
15	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
16	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
17	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
18	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

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19	4D Multimodal Nanomedicines Made of Nonequilibrium Auâ€“Fe Alloy Nanoparticles. ACS Nano, 2020, 14, 12840-12853.	7.3	53
20	Antenna triplet DFT calculations to drive the design of luminescent Ln³⁺complexes. Dalton Transactions, 2020, 49, 14556-14563.	1.6	7
21	Covalently Conjugated Goldâ€“Porphyrin Nanostructures. Nanomaterials, 2020, 10, 1644.	1.9	14
22	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
23	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
24	DFT modelling of the NO reduction process at the Cu-doped SrTiO3(1ÂŌÂ0) stepped surface. Inorganica Chimica Acta, 2020, 511, 119813.	1.2	2
25	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
26	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(<scp>ii</scp>) complexes. A thorough density functional theory â€“ energy decomposition analysis study. Dalton Transactions, 2019, 48, 12974-12985.	1.6	7
27	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
28	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
29	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
30	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
31	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
32	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
33	Reaction between Indazole and Pd-Bound Isocyanidesâ€”A Theoretical Mechanistic Study. Molecules, 2018, 23, 2942.	1.7	3
34	Substrate involvement in dioxygen bond dissociation catalysed by iron phthalocyanine supported on Ag(100). Chemical Communications, 2018, 54, 9418-9421.	2.2	13
35	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
36	On-Surface Synthesis of a Pure and Long-Range-Ordered Titanium(IV)-Porphyrin Contact Layer on Titanium Dioxide. Journal of Physical Chemistry C, 2017, 121, 13738-13746.	1.5	26

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37	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
38	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
39	Very high temperature tiling of tetraphenylporphyrin on rutile TiO₂(110). Nanoscale, 2017, 9, 11694-11704.	2.8	15
40	Pt(II) nitrile complexes: New insights on old complexes from a combined experimental and theoretical study. Inorganica Chimica Acta, 2017, 455, 489-504.	1.2	6
41	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
42	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
43	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
44	Tunable Band Alignment with Unperturbed Carrier Mobility of On-Surface Synthesized Organic Semiconducting Wires. ACS Nano, 2016, 10, 2644-2651.	7.3	40
45	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
46	Ligand-Field Strength and Symmetry-Restricted Covalency in CuIIComplexes - a Near-Edge X-ray Absorption Fine Structure Spectroscopy and Time-Dependent DFT Study. European Journal of Inorganic Chemistry, 2015, 2015, 2707-2713.	1.0	8
47	Hydrogen capture by porphyrins at the TiO₂(110) surface. Physical Chemistry Chemical Physics, 2015, 17, 30119-30124.	1.3	29
48	Moleculesâ€“Oligomersâ€“Nanowiresâ€“Graphene Nanoribbons: A Bottom-Up Stepwise On-Surface Covalent Synthesis Preserving Long-Range Order. Journal of the American Chemical Society, 2015, 137, 1802-1808.	6.6	221
49	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
50	XAS of tetrakis(phenyl)- and tetrakis(pentafluorophenyl)-porphyrin: an experimental and theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 2001-2011.	1.3	10
51	A theoretical study of the L3 pre-edge XAS in Cu(ii) complexes. Physical Chemistry Chemical Physics, 2014, 16, 19852-19855.	1.3	17
52	Double Level Selection in a Constitutional Dynamic Library of Coordination Driven Supramolecular Polygons. Inorganic Chemistry, 2014, 53, 7276-7287.	1.9	31
53	Stereoselective Photopolymerization of Tetraphenylporphyrin Derivatives on Ag(110) at the Subâ€Monolayer Level. Chemistry - A European Journal, 2014, 20, 14296-14304.	1.7	35
54	Electronic properties of CuPc and H2Pc: an experimental and theoretical study. Physical Chemistry Chemical Physics, 2013, 15, 12864.	1.3	51

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55	Electronic properties of tetrakis(pentafluorophenyl)porphyrin. New Journal of Chemistry, 2013, 37, 1036.	1.4	23
56	[Zn10(Î¼4-S)(Î¼3-S)6(Py)9(SO4)3] as a molecular model of ZnS surfaces: an experimental and theoretical study. Highlights in Theoretical Chemistry, 2013, , 161-168.	0.0	0
57	Tuning the catalytic activity of Ag(110)-supported Fe phthalocyanine in the oxygen reduction reaction. Nature Materials, 2012, 11, 970-977.	13.3	131
58	[Zn10(Âμ4-S)(Âμ3-S)6(Py)9(SO4)3] as a molecular model of ZnS surfaces: an experimental and theoretical study. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	0
59	Tetraphenylporphyrin electronic properties: a combined theoretical and experimental study of thin films deposited by SuMBD. Physical Chemistry Chemical Physics, 2010, 12, 871-880.	1.3	24
60	Role and effective treatment of dispersive forces in materials: Polyethylene and graphite crystals as test cases. Journal of Computational Chemistry, 2009, 30, 934-939.	1.5	653
61	Carbonyl copper(<scp>i</scp>) complexes with hydrotris(1,2,4-triazolyl)borate, hydrotris(pyrazolyl)borate, and tris(pyrazolyl)methaneligands: a DFT study. Physical Chemistry Chemical Physics, 2009, 11, 94-96.	1.3	6
62	Density Functional Theory Study of the Binding Capability of Tris(pyrazol-1-yl)methane toward Cu(I) and Ag(I) Cations. Journal of Physical Chemistry A, 2008, 112, 6723-6731.	1.1	9
63	Spinâ^'Orbit Relativistic Time-Dependent Density Functional Calculations of the Metal and Ligand Pre-Edge XAS Intensities of Organotitanium Complexes:â€‰ TiCl4, Ti(Î·5-C5H5)Cl3, and Ti(Î·5-C5H5)2Cl2. Journal of Physical Chemistry A, 2007, 111, 5270-5279.	1.1	54
64	A Theoretical Study of Amine Bonding in Titanium Alkoxide Adducts. Monatshefte FÃ¼r Chemie, 2007, 138, 1217-1223.	0.9	4
65	Experimental and QM/MM investigation of the hydrated silica surface reactivity. Chemical Physics Letters, 2005, 405, 459-464.	1.2	10
66	SO2 on TiO2(110) and Ti2O3(101Ì„2) Nonpolar Surfaces:â€‰ A DFT Study. Journal of Physical Chemistry B, 2005, 109, 12596-12602.	1.2	28
67	Spontaneous Self-Assembly of an Unsymmetric Trinuclear Triangular Copper(II) Pyrazolate Complex, [Cu3(Î¼3-OH)(Î¼-pz)3(MeCOO)2(Hpz)] (Hpz = Pyrazole). Synthesis, Experimental and Theoretical Characterization, Reactivity, and Catalytic Activity. Inorganic Chemistry, 2004, 43, 5865-5876.	1.9	117
68	A comparative study of the CO chemisorption on Ti2O3(102) and V2O3(102) non-polar surfaces. Surface Science, 2004, 566-568, 451-456.	0.8	6
69	A theoretical study of the interaction of CO2 with hydroxylated Î±-alumina. Surface Science, 2004, 566-568, 890-894.	0.8	8
70	Interstitial O3 in silica: a molecular cluster density functional study. Chemical Physics Letters, 2004, 392, 146-150.	1.2	2
71	A quasi-relativistic density functional study of structural and electronic properties of the bis-ketene cis-[Pt{Î·3-C3H5}{Î·1-C(PPh3)CO}2]+. Journal of Organometallic Chemistry, 2003, 682, 255-259.	0.8	3
72	A theoretical study of the electronic structure of O2 interstitial impurities in silica. Computational and Theoretical Chemistry, 2003, 631, 111-116.	1.5	2

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73	The organometallic chemistry of Ph3Pĩ…Cĩ…Cĩ…O.. Coordination Chemistry Reviews, 2003, 236, 15-33.	9.5	27
74	A theoretical study of the chemisorption of H2O and H2S on the Ti2O3(101Ì„2) non-polar surface. Physical Chemistry Chemical Physics, 2003, 5, 2461-2468.	1.3	9
75	Experimental and Theoretical Study of the Interaction of CO2with Î±-Al2O3. Inorganic Chemistry, 2003, 42, 436-445.	1.9	52
76	Further Insights into the Structure of [M(Î·2(C,Câ€˜)-C3O2)(PPh3)2] (M = Ni, Pd, Pt) by Quasi-Relativistic Density Functional Calculations and Solid-State CP/MAS NMR. Organometallics, 2002, 21, 2235-2239.	1.1	12
77	A Comparative Theoretical Investigation of Three Sodalite Systems:Â Cd4S(AlO2)6, Zn4O(BO2)6, and Zn4S(BO2)6. Journal of Physical Chemistry B, 2002, 106, 2569-2573.	1.2	8
78	A Comparative Study of CO Chemisorption on Al2O3and Ti2O3Nonpolar Surfaces. Journal of Physical Chemistry B, 2002, 106, 795-802.	1.2	31
79	UV-Photoelectron Spectra of [M(Î·3-C3H5)2] (M = Ni, Pd, Pt) Revisited:Â A Quasi-Relativistic Density Functional Study. Organometallics, 2001, 20, 754-762.	1.1	12
80	An experimental and theoretical study of the electronic and molecular structure of [Zn4(?4-S){Î¼-S2P(OC2H5)2}6]: the first molecular model of ZnS. Journal of Organometallic Chemistry, 2000, 593-594, 307-314.	0.8	8
81	Theoretical Study of the Chemisorption of CO on Al2O3(0001). Inorganic Chemistry, 2000, 39, 5232-5237.	1.9	24
82	Organometallic Chemistry of Ph3PCCO. Synthesis, Characterization, X-ray Structure Determination, and Density Functional Study of the First Stable Bis-Î·1-ketenyl Complex,trans-[PtCl2{Î·1-C(PPh3)CO}2]. Organometallics, 2000, 19, 1373-1383.	1.1	27
83	A theoretical study of the H2O and H2S chemisorption on Cu2O(111). Applied Surface Science, 1999, 142, 164-168.	3.1	44
84	A theoretical investigation of the relaxation effects induced on the ZnO(101Ì„0) surface by the chemisorption of H2 and CO. Applied Surface Science, 1999, 142, 192-195.	3.1	15
85	Density functional studies of molecular chemisorption on TiO2 (110). Applied Surface Science, 1999, 142, 196-199.	3.1	34
86	A comparative study of the NH3 chemisorption on ZnO(101Ì„0) and Cu2O(111) non-polar surfaces. Chemical Physics Letters, 1999, 300, 403-408.	1.2	23
87	Electronic structure of Nb impurities in and on TiO2. Physical Chemistry Chemical Physics, 1999, 1, 3793-3799.	1.3	20
88	Experimental and Theoretical Investigation of the Molecular and Electronic Structure of [Zn4(Î¼4-S){Î¼-S2As(CH3)2}6] and [Cd4(Î¼4-S){Î¼-S2As(CH3)2}6]:Â Two Possible Molecular Models of Extended Metal Chalcogenide Semiconductorsâ€. Inorganic Chemistry, 1999, 38, 1145-1152.	1.9	16
89	Theoretical Investigation of the Chemisorption of H2and CO on the ZnO(101Ì„0) Surface. Inorganic Chemistry, 1998, 37, 5482-5490.	1.9	26
90	Molecular Chemisorption on TiO2(110):Â A Local Point of View. Journal of Physical Chemistry B, 1998, 102, 10745-10752.	1.2	91

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91	An Experimental and Theoretical Study of the Electronic Structure of Zinc Thiophenolate-Capped Clusters. Inorganic Chemistry, 1997, 36, 4707-4716.	1.9	37
92	An LCAO-LDF study of the chemisorption of H2O and H2S on ZnO(0001) and ZnO(101Ì„0). Surface Science, 1997, 377-379, 587-591.	0.8	50
93	A theoretical study of the CO and NO chemisorption on Cu2O(111). Surface Science, 1997, 387, L1079-L1084.	0.8	32
94	A comparative study of CO and NO chemisorption on Cu2O(111) and Ag2O(111) non-polar surfaces. Chemical Physics Letters, 1997, 280, 53-58.	1.2	32
95	A molecular cluster approach to the study of the bonding of CO and NH3 to a d10 ion on ZnO(0001) and CuCl(111). Inorganica Chimica Acta, 1995, 235, 151-158.	1.2	15
96	Coordination chemistry of CO and NH3 on CuCl(111): an experimental and theoretical study of the CO and NH3 bonding to a d10 ion. Surface Science, 1994, 317, 422-436.	0.8	20
97	Coordination chemistry of CO and NH3 on ZnO(0001): a molecular cluster study of the CO and NH3 bonding interaction with a d10 ion. Surface Science, 1994, 303, 125-138.	0.8	34
98	A LCAO-LDF study of CO and NH3 chemisorption on ZnO(0001). Surface Science, 1994, 307-309, 1182-1187.	0.8	16
99	Zn4O(O2CNEt2)6: a further molecular model of ZnO. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 4363.	1.7	13
100	Hexakis(acetato)oxotetrazinc, a well-tailored molecular model of zinc oxide. An experimental and theoretical investigation of the electronic structure of Zn4O(acetate)6 and ZnO by means of UV and x-ray photoelectron spectroscopies and first principle local density molecular cluster calculations. Inorganic Chemistry, 1992, 31, 1558-1565.	1.9	130
101	Molecular orbital analysis of some ligand-bridged iron binuclear complexes by UV photoelectron spectroscopy and DV-Xî± calculations. Journal of Organometallic Chemistry, 1989, 366, 343-355.	0.8	14