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List of Publications by Year
in descending order

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101	2,883	218381	189595
papers	citations	26 h-index	50 g-index

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

#	Article	IF	Citations
1	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
2	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
3	Tuning the catalytic activity of Ag(110)-supported Fe phthalocyanine in the oxygen reduction reaction. Nature Materials, 2012, 11, 970-977.	13.3	131
4	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
5	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
6	Molecular Chemisorption on TiO2(110):Â A Local Point of View. Journal of Physical Chemistry B, 1998, 102, 10745-10752.	1.2	91
7	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
8	4D Multimodal Nanomedicines Made of Nonequilibrium Auâ€“Fe Alloy Nanoparticles. ACS Nano, 2020, 14, 12840-12853.	7.3	53
9	Experimental and Theoretical Study of the Interaction of CO2with Î±-Al2O3. Inorganic Chemistry, 2003, 42, 436-445.	1.9	52
10	Electronic properties of CuPc and H2Pc: an experimental and theoretical study. Physical Chemistry Chemical Physics, 2013, 15, 12864.	1.3	51
11	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
12	A theoretical study of the H2O and H2S chemisorption on Cu2O(111). Applied Surface Science, 1999, 142, 164-168.	3.1	44
13	Tunable Band Alignment with Unperturbed Carrier Mobility of On-Surface Synthesized Organic Semiconducting Wires. ACS Nano, 2016, 10, 2644-2651.	7.3	40
14	An Experimental and Theoretical Study of the Electronic Structure of Zinc Thiophenolate-Capped Clusters. Inorganic Chemistry, 1997, 36, 4707-4716.	1.9	37
15	Stereoselective Photopolymerization of Tetraphenylporphyrin Derivatives on Ag(110) at the Subâ€Monolayer Level. Chemistry - A European Journal, 2014, 20, 14296-14304.	1.7	35
16	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
17	Density functional studies of molecular chemisorption on TiO2 (110). Applied Surface Science, 1999, 142, 196-199.	3.1	34
18	A theoretical study of the CO and NO chemisorption on Cu2O(111). Surface Science, 1997, 387, L1079-L1084.	0.8	32

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19	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
20	A Comparative Study of CO Chemisorption on Al2O3and Ti2O3Nonpolar Surfaces. Journal of Physical Chemistry B, 2002, 106, 795-802.	1.2	31
21	Double Level Selection in a Constitutional Dynamic Library of Coordination Driven Supramolecular Polygons. Inorganic Chemistry, 2014, 53, 7276-7287.	1.9	31
22	Hydrogen capture by porphyrins at the TiO₂(110) surface. Physical Chemistry Chemical Physics, 2015, 17, 30119-30124.	1.3	29
23	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
24	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
25	The organometallic chemistry of Ph3P˜...C˜...C˜...O.. Coordination Chemistry Reviews, 2003, 236, 15-33.	9.5	27
26	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
27	Theoretical Investigation of the Chemisorption of H2and CO on the ZnO(101Ì„0) Surface. Inorganic Chemistry, 1998, 37, 5482-5490.	1.9	26
28	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
29	Theoretical Study of the Chemisorption of CO on Al2O3(0001). Inorganic Chemistry, 2000, 39, 5232-5237.	1.9	24
30	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
31	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
32	Electronic properties of tetrakis(pentafluorophenyl)porphyrin. New Journal of Chemistry, 2013, 37, 1036.	1.4	23
33	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
34	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
35	Electronic structure of Nb impurities in and on TiO2. Physical Chemistry Chemical Physics, 1999, 1, 3793-3799.	1.3	20
36	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

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37	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
38	A theoretical study of the L3 pre-edge XAS in Cu(ii) complexes. Physical Chemistry Chemical Physics, 2014, 16, 19852-19855.	1.3	17
39	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
40	A LCAO-LDF study of CO and NH3 chemisorption on ZnO(0001). Surface Science, 1994, 307-309, 1182-1187.	0.8	16
41	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
42	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
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	Ferrous to Ferric Transition in Feâ€Phthalocyanine Driven by NO₂ Exposure. Chemistry - A European Journal, 2021, 27, 3526-3535.	1.7	16
45	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
46	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
47	Very high temperature tiling of tetraphenylporphyrin on rutile TiO₂(110). Nanoscale, 2017, 9, 11694-11704.	2.8	15
48	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
49	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
50	Covalently Conjugated Goldâ€“Porphyrin Nanostructures. Nanomaterials, 2020, 10, 1644.	1.9	14
51	Zn4O(O2CNEt2)6: a further molecular model of ZnO. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 4363.	1.7	13
52	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
53	Substrate involvement in dioxygen bond dissociation catalysed by iron phthalocyanine supported on Ag(100). Chemical Communications, 2018, 54, 9418-9421.	2.2	13
54	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

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55	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
56	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
57	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
58	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
59	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
60	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
61	Experimental and QM/MM investigation of the hydrated silica surface reactivity. Chemical Physics Letters, 2005, 405, 459-464.	1.2	10
62	XAS of tetrakis(phenyl)- and tetrakis(pentafluorophenyl)-porphyrin: an experimental and theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 2001-2011.	1.3	10
63	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
64	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
65	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
66	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
67	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
68	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
69	A theoretical study of the interaction of CO2 with hydroxylated Î±-alumina. Surface Science, 2004, 566-568, 890-894.	0.8	8
70	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
71	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
72	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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73	Antenna triplet DFT calculations to drive the design of luminescent Ln³⁺complexes. Dalton Transactions, 2020, 49, 14556-14563.	1.6	7
74	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
75	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
76	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
77	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
78	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
79	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
80	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
81	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
82	Distortion-driven spin switching in electron-doped metal porphyrins. Journal of Materials Chemistry C, 2022, 10, 9748-9757.	2.7	5
83	A Theoretical Study of Amine Bonding in Titanium Alkoxide Adducts. Monatshefte FÃ¼r Chemie, 2007, 138, 1217-1223.	0.9	4
84	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
85	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
86	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
87	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
88	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
89	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
90	Reaction between Indazole and Pd-Bound Isocyanidesâ€”A Theoretical Mechanistic Study. Molecules, 2018, 23, 2942.	1.7	3

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91	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
92	Stabilization of high-spin Mn ions in tetra-pyrrolic configuration on copper. Applied Surface Science, 2021, 551, 149307.	3.1	3
93	A theoretical study of the electronic structure of O2 interstitial impurities in silica. Computational and Theoretical Chemistry, 2003, 631, 111-116.	1.5	2
94	Interstitial O3 in silica: a molecular cluster density functional study. Chemical Physics Letters, 2004, 392, 146-150.	1.2	2
95	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
96	DFT modelling of the NO reduction process at the Cu-doped SrTiO3(1Â0Â0) stepped surface. Inorganica Chimica Acta, 2020, 511, 119813.	1.2	2
97	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
98	[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
99	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
100	[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
101	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