Athanassios C Tsipis

List of Publications by Year
in descending order

101	2,496	218677	223800
papers	citations	26 h-index	46 g-index

109	109	109	3301
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Selective capture of hexavalent chromium from an anion-exchange column of metal organic resinâ€“alginic acid composite. Chemical Science, 2016, 7, 2427-2436.	7.4	158
2	All in one porous material: exceptional sorption and selective sensing of hexavalent chromium by using a Zr⁴⁺ MOF. Journal of Materials Chemistry A, 2017, 5, 14707-14719.	10.3	150
3	Hydrometal Analogues of Aromatic Hydrocarbons:Â A New Class of Cyclic Hydrocoppers(I). Journal of the American Chemical Society, 2003, 125, 1136-1137.	13.7	118
4	Copper(I) Halide Complexes with 1,3-Propanebis(diphenylphosphine) and Heterocyclic Thione Ligands:Â Crystal and Electronic Structures (DFT) of [CuCl(pymtH)(dppp)], [CuBr(pymtH)(dppp)], and [Cu(Î¼-I)(dppp)]2. Inorganic Chemistry, 2002, 41, 6875-6886.	4.0	104
5	Aromatic Gold and Silver â€˜Rings':Â Hydrosilver(I) and Hydrogold(I) Analogues of Aromatic Hydrocarbons. Journal of the American Chemical Society, 2004, 126, 12916-12929.	13.7	98
6	Experimental and Theoretical Study of the Antisymmetric Magnetic Behavior of Copper inverse-9-Metallacrown-3 Compounds. Inorganic Chemistry, 2008, 47, 7545-7555.	4.0	71
7	Alkaline Earth Metal Ion/Dihydroxyâ€“Terephthalate MOFs: Structural Diversity and Unusual Luminescent Properties. Inorganic Chemistry, 2015, 54, 5813-5826.	4.0	71
8	The Role of the 5f Orbitals in Bonding, Aromaticity, and Reactivity of Planar Isocyclic and Heterocyclic Uranium Clusters. Journal of the American Chemical Society, 2008, 130, 9144-9155.	13.7	69
9	Efficiency of the NICSzz-scan curves to probe the antiaromaticity of organic and inorganic rings/cages. Physical Chemistry Chemical Physics, 2009, 11, 8244.	2.8	68
10	Exceptional TcO₄^{â^’} sorption capacity and highly efficient ReO₄^{â^’} luminescence sensing by Zr⁴⁺ MOFs. Journal of Materials Chemistry A, 2018, 6, 20813-20821.	10.3	54
11	Structure, Energetics, and Bonding of First Row Transition Metal Pentazolato Complexes:Â A DFT Study. Inorganic Chemistry, 2004, 43, 1273-1286.	4.0	48
12	DNA interaction studies and evaluation of biological activity of homo- and hetero-trihalide mononuclear Cu(II) Schiff base complexes. Quantitative structureâ€“activity relationships. Journal of Inorganic Biochemistry, 2008, 102, 1749-1764.	3.5	45
13	Ligand-Stabilized Aromatic Three-Membered Gold Rings and Their Sandwichlike Complexes. Journal of the American Chemical Society, 2005, 127, 10623-10638.	13.7	43
14	3d/4f Coordination Clusters as Cooperative Catalysts for Highly Diastereoselective Michael Addition Reactions. Inorganic Chemistry, 2017, 56, 9563-9573.	4.0	43
15	Synthesis of Homo- or Hetero-trinuclear Palladium(II)/Platinum(II) Compounds with Bridging Phosphido Ligands. Crystal and Electronic Structures (DFT) of [N(PPh3)2]2[Pt3(Î¼-PPh2)4(C6F5)4] and of Its Oxidation Product [Pt3(C6F5)4(Î¼-PPh2)4]â€. Organometallics, 2001, 20, 5571-5582.	2.3	40
16	Electronic Structure and Optical Properties of Mixed Phenylene Vinylene/Phenylene Ethynylene Conjugated Oligomers. Chemistry of Materials, 2002, 14, 1362-1368.	6.7	38
17	Formation of PPh2C6F5through Phosphido Platinum and/or Palladium(III) Intermediatesâ€“,âŠ¥. Organometallics, 2006, 25, 1084-1091.	2.3	38
18	Accurate prediction of ¹⁹⁵Pt NMR chemical shifts for a series of Pt(<scp>ii</scp>) and Pt(<scp>iv</scp>) antitumor agents by a non-relativistic DFT computational protocol. Dalton Transactions, 2014, 43, 5409-5426.	3.3	36

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19	Experimental and Quantum Chemical Study of the Mechanism of an Unexpected Intramolecular Reductive Coupling of a Bridging Phosphido Ligand and a C6F5Group and the Reversible Oxidative Addition of PPh2C6F5#,â€–. Organometallics, 2004, 23, 1797-1810.	2.3	35
20	DFT/TDDFT insights into the chemistry, biochemistry and photophysics of copper coordination compounds. RSC Advances, 2014, 4, 32504-32529.	3.6	33
21	Diagnosis of the Ïƒ-, Ï€- and (Ïƒ+Ï€)-Aromaticity by the Shape of the NICSzz-Scan Curves and Symmetry-Based Selection Rules. Symmetry, 2010, 2, 284-319.	2.2	32
22	Oxidative Addition of Halogens to Homoleptic Perfluoromethyl or Perfluorophenyl Derivatives of Platinum(II): A Comparative Study. Chemistry - A European Journal, 2009, 15, 6371-6382.	3.3	28
23	Oxidovanadium(IV/V) Complexes as New Redox Mediators in Dye-Sensitized Solar Cells: A Combined Experimental and Theoretical Study. Inorganic Chemistry, 2015, 54, 3979-3988.	4.0	28
24	One-Pot and Step-by-Step N-Assisted C_{Ph}â^'H Activation in 2-(4-Bromophenyl)imidazol[1,2-a]pyridine: Synthesis of a New C,N-Cyclometalated Compound [{Pt(C^{â^§}N)(Î¼-Cl)}₂] as Precursor of Luminescent Platinum(II) Compounds. Organometallics, 2010, 29, 1396-1405.	2.3	25
25	An Exploration of the Structural and Bonding Variability in Mixed-Ligand Benzimidazole-2-thione(bromo)(triarylphosphane)dicopper(I) Complexes with Diamond-Shaped Cu2(?-X)2 Core Structures. European Journal of Inorganic Chemistry, 2005, 2005, 1442-1452.	2.0	24
26	All-Organometallic Analogues of Zeise's Salt for the Three Group 10 Metals. Organometallics, 2005, 24, 3539-3546.	2.3	24
27	Mechanistic aspects of the complete set of hydrolysis and anation reactions of cis - and trans -DDP related to their antitumor activity modeled by an improved ASED-MO approach. Computational and Theoretical Chemistry, 2002, 584, 235-248.	1.5	23
28	First light-emitting electrochemical cell with [Ag(<scp>i</scp>)(N^N)(P^P)] type complex. RSC Advances, 2015, 5, 95047-95053.	3.6	21
29	Molecular geometries, electronic structures and energetics of neutral and cationic mono-ligated ammonia complexes of the d-block elements calculated by an improved modified ASED[ndash]MO model. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 11-24.	1.7	20
30	Structural and Spectroscopic Properties of New Copper(I) Complexes with 1,1,1â€Tris(diphenylphosphanylmethyl)ethane and Heterocyclic Thiolates. European Journal of Inorganic Chemistry, 2008, 2008, 5029-5037.	2.0	20
31	Cobalt(<scp>ii</scp>/<scp>iii</scp>), nickel(<scp>ii</scp>) and copper(<scp>ii</scp>) coordination clusters employing a monoanionic Schiff base ligand: synthetic, topological and computational mechanistic aspects. CrystEngComm, 2015, 17, 6753-6764.	2.6	20
32	Shedding light on the use of Cu(<scp>ii</scp>)-salen complexes in the A³ coupling reaction. Dalton Transactions, 2020, 49, 289-299.	3.3	20
33	A new class of â€œall-metalâ€•aromatic hydrido-bridged binary coinage metal heterocycles. A DFT study. New Journal of Chemistry, 2007, 31, 852-859.	2.8	19
34	Synthesis and Characterization of the Double Salts [Pt(bzq)(CNR)₂][Pt(bzq)(CN)₂] with Significant PtÂ·Â·Â·Pt and Ï€Â·Â·Â·Ï€ Interactions. Mechanistic Insights into the Ligand Exchange Process from Joint Experimental and DFT Study. Organometallics, 2012, 31, 2729-2740.	2.3	19
35	Ab initio and density functional electronic structure study of molybdenum oxide clusters. Physical Chemistry Chemical Physics, 2000, 2, 1357-1363.	2.8	18
36	Molecular Transition Metal Oxides:â€‰ Ab Initio and Density Functional Electronic Structure Study of Tungsten Oxide Clusters. Journal of Physical Chemistry A, 2000, 104, 859-865.	2.5	18

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37	Exploring the Forces That Control the Pâ”C Bond Length in Phosphamides and Their Complexes:Â The Key Role of Hyperconjugation. Organometallics, 2006, 25, 2774-2781.	2.3	18
38	Unveiling the Nature of Binding Interactions of Acetylene and Ethylene with Triangular Coinage Metal Clusters: A DFT Computational Study. Organometallics, 2010, 29, 354-363.	2.3	18
39	Diagnosis of magnetoresponsive aromatic and antiaromatic zones in threeâ€membered rings of dâ€ and fâ€block elements. Journal of Computational Chemistry, 2010, 31, 431-446.	3.3	17
40	Aquanitrato Complexes of Palladium, Rhodium, and Platinum: A Comparative 15 N NMR and DFT Study. European Journal of Inorganic Chemistry, 2018, 2018, 627-639.	2.0	17
41	A theoretical study of molecular titanium oxide clusters: structure, bonding, vibrations and stability. Physical Chemistry Chemical Physics, 1999, 1, 4453-4458.	2.8	16
42	An Experimental and Density Functional Study of the Interaction of CuII Complexes of Diethylenetriamine (Dien) with Pyridine, Nicotinic Acid, and Nicotinamide: The Crystal Structure of [Cu(dien)(nicotinamide)(NO3)2]. European Journal of Inorganic Chemistry, 2006, 2006, 2083-2095.	2.0	16
43	Building trans-philicity (trans-effect/trans-influence) ladders for octahedral complexes by using an NMR probe. Dalton Transactions, 2019, 48, 1814-1822.	3.3	16
44	Alkylamino-terephthalate ligands stabilize 8-connected Zr⁴⁺ MOFs with highly efficient sorption for toxic Se species. Journal of Materials Chemistry A, 2021, 9, 3379-3387.	10.3	16
45	Synthesis and Reactivity of the Unsaturated Trinuclear Phosphanido Complex [(C₆F₅)₂Pt(Î¼-PPh₂)₂Pt(Î¼-PPh₂)₂Pt(PPh₂)₂]. Inorganic Chemistry, 2013, 52, 1942-1953.	4.6	15
46	Synthesis, structural and physicochemical characterization of a new type Ti₆-oxo cluster protected by a cyclic imide dioxime ligand. Dalton Transactions, 2019, 48, 5551-5559.	3.3	15
47	From a 44-electron to a 48-electron trinuclear phosphido platinum complex: density functional study of [{(CF3)(PH3)Pt(Î¼-PH2)(Î¼-H)}2Pt] and [{(CF3)(PH3)Pt(Î¼-PH2)(Î¼-I)}2Pt] model compounds. Inorganica Chimica Acta, 2005, 358, 1377-1385.	2.4	14
48	Transâ€philicity (transâ€influence/transâ€effect) ladders for square planar platinum(II) complexes constructed by ³⁵Cl NMR probe. Journal of Computational Chemistry, 2019, 40, 2550-2562.	3.3	14
49	DFT insights into the photocatalytic reduction of CO₂ to CO by Re(<scp>i</scp>) complexes: the crucial role of the triethanolamine â€œmagicâ€•sacrificial electron donor. Dalton Transactions, 2021, 50, 14797-14809.	3.3	13
50	Synthesis and Characterization of New Five-Coordinate Platinum Nitrosyl Derivatives: Density Functional Theory Study of Their Electronic Structure. Chemistry - A European Journal, 2003, 9, 4094-4105.	3.3	12
51	Theoretical Study on the Mechanism of Reaction of Ground-State Fe Atoms with Carbon Dioxide. Collection of Czechoslovak Chemical Communications, 2004, 69, 13-33.	1.0	12
52	Unraveling the Origin of the Peculiar Reaction Field of Triruthenium Ring Core Structures. Journal of the American Chemical Society, 2007, 129, 13905-13922.	13.7	12
53	Shedding Light on Intermolecular Metalâ€“Organic Ring Interactions by Theoretical Studies. ChemPlusChem, 2012, 77, 354-360.	2.8	12
54	Molecular and Electronic Structure, Magnetotropicity and Absorption Spectra of Benzeneâ€“Trinuclear Copper(I) and Silver(I) Trihalide Columnar Binary Stacks. Inorganic Chemistry, 2012, 51, 2541-2559.	4.0	11

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55	Face-to-Face Stacks of Trinuclear Gold(I) Trihalides with Benzene, Hexafluorobenzene, and Borazine: Impact of Aromaticity on Stacking Interactions. Inorganic Chemistry, 2013, 52, 1047-1060.	4.0	11
56	Highly Efficient Sorption of Methyl Orange by a Metalâ€“Organic Resinâ€“Alginic Acid Composite. ChemPlusChem, 2017, 82, 1188-1196.	2.8	11
57	Quantum chemical study of the coordination of glycolic acid conformers and their conjugate bases to [Ca(OH2)n]2+ (n=0â€“4) ions. Computational and Theoretical Chemistry, 2003, 630, 81-100.	1.5	10
58	Synthesis, structural and theoretical studies of a rare hexameric water cluster held in the lattice of {[Zn(HL)(phen)(H2O)]â˜™3(H2O)}2 (H3L=trans-aconitic acid). Inorganic Chemistry Communication, 2011, 14, 87-91.	3.9	10
59	Loading Aromatic Six-Membered Carbocyclic Rings with Coinage Metals: Aromatic Metalated Benzenes C6M6 and 1,3,5-C6H3M3 (M = Cu, Ag, Au) Exhibiting Intriguing Properties. Organometallics, 2012, 31, 7206-7212.	2.3	10
60	Accurate prediction of ¹⁹⁵Pt-NMR chemical shifts for hydrolysis products of [PtCl₆]^{2â˜’} in acidic and alkaline aqueous solutions by non-relativistic DFT computational protocols. Journal of Coordination Chemistry, 2015, 68, 3788-3804.	2.2	10
61	Ab Initio Quantum Chemical Study of the Coordination Preferences and Catalytic Role of Cu+ Ions in the Dehydration Reactions of Hydroxyformaldoxime Conformers and the Oxidation of HCN to Hydroxyformaldoxime by Hydrogen Peroxide. Journal of Physical Chemistry A, 2002, 106, 1425-1440.	2.5	9
62	Prediction of ¹⁹⁵Pt NMR of photoactivable diazidoâ€•and azineâ€Pt(IV) anticancer agents by DFT computational protocols. Magnetic Resonance in Chemistry, 2017, 55, 145-153.	1.9	9
63	Design and Assembly of Covalently Functionalised Polyoxofluorovanadate Molecular Hybrids. Chemistry - A European Journal, 2018, 24, 3836-3845.	3.3	9
64	Synthesis, characterization, DNA-binding properties and electronic structure (DFT) of ruthenium oligopyridine complexes. Inorganic Chemistry Communication, 2008, 11, 1341-1346.	3.9	8
65	Structural, electronic, bonding, magnetic, and optical properties of bimetallic [Ru_nAu_m]^{0/+} (n + m â‰¤ 3) clusters. Journal of Computational Chemistry, 2010, 31, 2836-2852.	3.3	8
66	Structural, electronic, and magnetoresponsive properties of triangular lanthanide clusters and their freeâ€standing nitrides. Journal of Computational Chemistry, 2011, 32, 620-638.	3.3	7
67	Synthesis, Bonding, and Reactivity of Vanadium(IV) Oxidoâ€“Fluorido Compounds with Neutral Chelate Ligands of the General Formula cis-[V^{IV}(â•O)(F)(L_{Nâ€“N})₂]⁺. Inorganic Chemistry, 2016, 55, 1364-1366.	4.0	7
68	Synthesis, Structural, and Physicochemical Characterization of a Ti₆ and a Unique Type of Zr₆ Oxo Clusters Bearing an Electron-Rich Unsymmetrical {OON} Catecholate/Oxime Ligand and Exhibiting Metalloaromaticity. Inorganic Chemistry, 2020, 59, 18345-18357.	4.0	7
69	NMR probe effects on trans-philicity and trans-influence ladders in square planar Pt(<scp>II</scp>) complexes. New Journal of Chemistry, 2020, 44, 7976-7986.	2.8	7
70	Deciphering the bonding mode of the trihalide ligands in a series of halogen carrier homo- and hetero-trihalide Cu(II) Schiff base complexes. Polyhedron, 2008, 27, 289-298.	2.2	6
71	Probing the electronic structure, chemical bonding, and excitation spectra of [CuE]^{+/0/â˜’} (E = 14 group element) diatomics employing DFT and ab initio methods. Journal of Computational Chemistry, 2012, 33, 2318-2331.	3.3	6
72	Shedding light on the bonding, photophysical and magnetotropic properties of triangular Pt3complexes and their â€œopen-faceâ€•TlPt3half-sandwiches. Dalton Transactions, 2013, 42, 2201-2212.	3.3	6

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73	The molecular, electronic, bonding, and photophysical features of the [(c-Pt3)Tl(c-Pt3)]+ inorganic metallocenes. Dalton Transactions, 2013, 42, 8307.	3.3	6
74	Sequential metalation of benzene: electronic, bonding, magnetotropic and spectroscopic properties of coinage metalated benzenes studied by DFT. Journal of Molecular Modeling, 2015, 21, 153.	1.8	6
75	Prediction of 195 Pt NMR chemical shifts of dissolution products of H2 [Pt(OH)6] in nitric acid solutions by DFT methods: how important are the counter-ion effects?. Magnetic Resonance in Chemistry, 2016, 54, 656-664.	1.9	6
76	Synthesis of new photosensitive H₂BBQ²⁺[ZnCl₄]^{2â¯}/[(ZnCl)₂(Î¼-BBH)] complexes, through selective oxidation of H₂O to H₂O₂. Dalton Transactions, 2017, 46, 3688-3699.	3.3	6
77	Density functional study of configurational, conformational, energetic, electronic and spectroscopic properties of fluorohydroxyformaldoxime and its dehydration products. Physical Chemistry Chemical Physics, 1999, 1, 4541-4547.	2.8	5
78	Conformational preferences, rotational barriers and energetics of purine nucleobase rotation and dissociation in square planar platinum(II) antitumour complexes: Structureâ€“activity correlation. Physical Chemistry Chemical Physics, 2001, 3, 5165-5172.	2.8	5
79	Binding of cerium monoxide to annulenes and buckybowls. Physical Chemistry Chemical Physics, 2012, 14, 14917.	2.8	5
80	Interaction of Elemental Mercury with a Diverse Series of Ï€-Organic Substrates Probed by Computational Methods: Is Mercury Fixation Possible?. ACS Earth and Space Chemistry, 2018, 2, 451-461.	2.7	5
81	Dinuclear and Mononuclear Rhenium Coordination Compounds upon Employment of a Schiff-Base Triol Ligand: Structural, Magnetic, and Computational Studies. Inorganic Chemistry, 2019, 58, 8596-8606.	4.0	5
82	Upright or In-Plane Conformational Preference: Dilemma of Î·2-Coordinated Câ•C Double Bond in PtX2(CO)(Î·2-ene) (X = H, Cl, or C6F5) Complexes. Organometallics, 2008, 27, 3701-3713.	2.3	4
83	Structure and properties of a rhodium(III) pentanitrato complex embracing uni- and bidentate nitrato ligands. Polyhedron, 2018, 147, 69-74.	2.2	4
84	Polynuclear ampyrone based 3d coordination clusters. CrystEngComm, 2018, 20, 1411-1421.	2.6	4
85	Electronic structure calculations on multiply charged anions containing Mï£¿S bonds (M = Cr, Mo, W) and their heterobimetallic cluster complexes. International Journal of Quantum Chemistry, 2007, 107, 418-439.	2.0	3
86	Modeling the cysteamine catalyzed cysteine proteinases using DFT: mechanistic insights into the hydrolysis of acetyl-p-nitroanilide. New Journal of Chemistry, 2013, 37, 4061.	2.8	3
87	Influence of the metal salt on the self-assembly of isophthaloylbis-Î²-alanine and Cu(II) ion. Polyhedron, 2015, 89, 313-321.	2.2	3
88	Electronic, bonding, and optical properties of 1d [<scp>C</scp>u<scp>CN</scp>]_n (nâ€‰=â€‰1â€“10) chains, 2d [<scp>C</scp>u<scp>CN</scp>]_n (nâ€‰=â€‰2â€“10) nanorings, and 3d [<scp>C</scp>u_n(<scp>CN</scp>)_n]_m (nâ€‰=â€‰4, mâ€‰=â€‰2, 3; nâ€‰=â€‰10, mâ€‰=â€‰2) tubes studied by DFT/TDâ€DFT methods. Computational Chemistry, 2015, 36, 1334-1347.	3.3	3
89	cis- and trans-Ligand Effects on the Inverse trans-Influence in [U^{VI}(O)(L)Cl₄]^{0/â€“} (L = Unidentate Ligand) Complexes. Inorganic Chemistry, 2020, 59, 8946-8959.	4.0	3
90	Mechanistic aspects of the dehydration and dehydrohalogenation of halo-hydroxyformaldoxime conformers. A quantum chemical model study. Journal of Computational Chemistry, 2002, 23, 1266-1280.	3.3	2

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91	DFT assessment of the spectroscopic constants and absorption spectra of neutral and charged diatomic species of group 11 and 14 elements. Journal of Computational Chemistry, 2014, 35, 1762-1777.	3.3	2
92	Trans ligand effects on 195Pt NMR shielding constants of square planar Pt(II) complexes. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	2
93	Anomeric and Perlin Effect Ladders for 2-Substituted 2-Fluorotetrahydro-2H-pyrans Using Sensitive Structural, Energetic, and NMR Probes. Journal of Physical Chemistry A, 2021, 125, 7457-7472.	2.5	2
94	Density Functional Study of the Electronic Structure and Related Properties of Pt(NO)/Pt(NO2) Redox Couples. Collection of Czechoslovak Chemical Communications, 2003, 68, 423-446.	1.0	1
95	Mimicking the electronic structure of endohedral triangular lanthanide clusters in â€œfreeâ€•from host carbon cages metallofullerenes uncovers a peculiar reactivity pattern. Journal of Coordination Chemistry, 2014, 67, 2550-2563.	2.2	1
96	The hydrogen storage capacity of coinage metalated benzenes studied by DFT. Journal of Coordination Chemistry, 2015, 68, 2653-2665.	2.2	1
97	¹⁹⁵Pt NMR parameters as strong descriptors in oneâ€parameter QSAR models for platinumâ€based antitumor compounds. Magnetic Resonance in Chemistry, 2017, 55, 662-669.	1.9	1
98	DFT study of coinage metal-hydrogen associations as hydrogen storage materials stabilized by weakly coordinating anions. International Journal of Hydrogen Energy, 2019, 44, 8341-8346.	7.1	1
99	Probing the electronic structure, magnetotropicity, and absorption spectra of benzene trapped by lanthanide monoxides, C₆H₆Â·Â·Â·LnO, using DFT methods. International Journal of Quantum Chemistry, 2013, 113, 694-708.	2.0	0
100	Exploring possible reaction pathways for the oâ€atom transfer reactions to unsaturated substrates catalyzed by a [Niâ€NO₂] â†” [Niâ€NO] redox couple using DFT methods. Journal of Computational Chemistry, 2017, 38, 1780-1788.	3.3	0
101	Investigating the isolation and interconversion of two diastereoisomers in an octahedral system. New Journal of Chemistry, 2019, 43, 17141-17145.	2.8	0