# 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 | Alkylamino-terephthalate ligands stabilize 8-connected Zr<sup>4+</sup> MOFs with highly efficient sorption for toxic Se species. Journal of Materials Chemistry A, 2021, 9, 3379-3387. | 10.3 | 16 |
| 2 | DFT insights into the photocatalytic reduction of CO<sub>2</sub> 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 |
| 3 | 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 |
| 4 | Shedding light on the use of Cu(<scp>ii</scp>)-salen complexes in the A<sup>3</sup> coupling reaction. Dalton Transactions, 2020, 49, 289-299. | 3.3 | 20 |
| 5 | Trans ligand effects on 195Pt NMR shielding constants of square planar Pt(II) complexes. Theoretical Chemistry Accounts, 2020, 139, 1. | 1.4 | 2 |
| 6 | Synthesis, Structural, and Physicochemical Characterization of a Ti<sub>6</sub> and a Unique Type of Zr<sub>6</sub> Oxo Clusters Bearing an Electron-Rich Unsymmetrical {OON} Catecholate/Oxime Ligand and Exhibiting Metalloaromaticity. Inorganic Chemistry, 2020, 59, 18345-18357. | 4.0 | 7 |
| 7 | 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 |
| 8 | cis- and trans-Ligand Effects on the Inverse trans-Influence in [U<sup>VI</sup>(O)(L)Cl<sub>4</sub>]<sup>0/â€“</sup> (L = Unidentate Ligand) Complexes. Inorganic Chemistry, 2020, 59, 8946-8959. | 4.0 | 3 |
| 9 | Transâ€philicity (transâ€influence/transâ€effect) ladders for square planar platinum(II) complexes constructed by <sup>35</sup>Cl NMR probe. Journal of Computational Chemistry, 2019, 40, 2550-2562. | 3.3 | 14 |
| 10 | 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 |
| 11 | 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 |
| 12 | 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 |
| 13 | Synthesis, structural and physicochemical characterization of a new type Ti<sub>6</sub>-oxo cluster protected by a cyclic imide dioxime ligand. Dalton Transactions, 2019, 48, 5551-5559. | 3.3 | 15 |
| 14 | Investigating the isolation and interconversion of two diastereoisomers in an octahedral system. New Journal of Chemistry, 2019, 43, 17141-17145. | 2.8 | 0 |
| 15 | Structure and properties of a rhodium(III) pentanitrato complex embracing uni- and bidentate nitrato ligands. Polyhedron, 2018, 147, 69-74. | 2.2 | 4 |
| 16 | Polynuclear ampyrone based 3d coordination clusters. CrystEngComm, 2018, 20, 1411-1421. | 2.6 | 4 |
| 17 | Design and Assembly of Covalently Functionalised Polyoxofluorovanadate Molecular Hybrids. Chemistry - A European Journal, 2018, 24, 3836-3845. | 3.3 | 9 |
| 18 | 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 |

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|---|---|---|---|
| 19 | 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 |
| 20 | Exceptional TcO<sub>4</sub><sup>â^'</sup> sorption capacity and highly efficient ReO<sub>4</sub><sup>â^'</sup> luminescence sensing by Zr<sup>4+</sup> MOFs. Journal of Materials Chemistry A, 2018, 6, 20813-20821. | 10.3 | 54 |
| 21 | <sup>195</sup>Pt 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 |
| 22 | Synthesis of new photosensitive H<sub>2</sub>BBQ<sup>2+</sup>[ZnCl<sub>4</sub>]<sup>2â^'</sup>/[(ZnCl)<sub>2</sub>(Î¼-BBH)] complexes, through selective oxidation of H<sub>2</sub>O to H<sub>2</sub>O<sub>2</sub>. Dalton Transactions, 2017, 46, 3688-3699. | 3.3 | 6 |
| 23 | Exploring possible reaction pathways for the oâ€atom transfer reactions to unsaturated substrates catalyzed by a [Niâ€NO<sub>2</sub>] â†" [Niâ€NO] redox couple using DFT methods. Journal of Computational Chemistry, 2017, 38, 1780-1788. | 3.3 | 0 |
| 24 | All in one porous material: exceptional sorption and selective sensing of hexavalent chromium by using a Zr<sup>4+</sup> MOF. Journal of Materials Chemistry A, 2017, 5, 14707-14719. | 10.3 | 150 |
| 25 | Highly Efficient Sorption of Methyl Orange by a Metalâ€"Organic Resinâ€"Alginic Acid Composite. ChemPlusChem, 2017, 82, 1188-1196. | 2.8 | 11 |
| 26 | 3d/4f Coordination Clusters as Cooperative Catalysts for Highly Diastereoselective Michael Addition Reactions. Inorganic Chemistry, 2017, 56, 9563-9573. | 4.0 | 43 |
| 27 | Prediction of <sup>195</sup>Pt 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 |
| 28 | 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 |
| 29 | Synthesis, Bonding, and Reactivity of Vanadium(IV) Oxidoâ€"Fluorido Compounds with Neutral Chelate Ligands of the General Formula cis-[V<sup>IV</sup>(â•O)(F)(L<sub>Nâ€"N</sub>)<sub>2</sub>]<sup>+</sup>. Inorganic Chemistry, 2016, 55, 1364-1366. | 4.0 | 7 |
| 30 | 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 |
| 31 | Accurate prediction of <sup>195</sup>Pt-NMR chemical shifts for hydrolysis products of [PtCl<sub>6</sub>]<sup>2â^'</sup> in acidic and alkaline aqueous solutions by non-relativistic DFT computational protocols. Journal of Coordination Chemistry, 2015, 68, 3788-3804. | 2.2 | 10 |
| 32 | 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 |
| 33 | 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 |
| 34 | Alkaline Earth Metal Ion/Dihydroxyâ€"Terephthalate MOFs: Structural Diversity and Unusual Luminescent Properties. Inorganic Chemistry, 2015, 54, 5813-5826. | 4.0 | 71 |
| 35 | 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 |
| 36 | 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 |

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|---|---|---|---|
| 37 | Structure, bonding, and optical properties of 1d [<scp>C</scp>u<scp>CN</scp>]<sub>n</sub> (nâ€‰=â€‰1â€“10) chains, 2d [<scp>C</scp>u<scp>CN</scp>]<sub>n</sub> (nâ€‰=â€‰2â€“10) nanorings, and 3d [<scp>C</scp>u<sub>n</sub>(<scp>CN</scp>)<sub>n</sub>]<sub>m</sub> (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 |
| 38 | The hydrogen storage capacity of coinage metalated benzenes studied by DFT. Journal of Coordination Chemistry, 2015, 68, 2653-2665. | 2.2 | 1 |
| 39 | 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 |
| 40 | 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 |
| 41 | Accurate prediction of <sup>195</sup>Pt 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 |
| 42 | 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 |
| 43 | DFT/TDDFT insights into the chemistry, biochemistry and photophysics of copper coordination compounds. RSC Advances, 2014, 4, 32504-32529. | 3.6 | 33 |
| 44 | Probing the electronic structure, magnetotropicity, and absorption spectra of benzene trapped by lanthanide monoxides, C<sub>6</sub>H<sub>6</sub>Â·Â·Â·LnO, using DFT methods. International Journal of Quantum Chemistry, 2013, 113, 694-708. | 2.0 | 0 |
| 45 | 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 |
| 46 | 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 |
| 47 | 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 |
| 48 | The molecular, electronic, bonding, and photophysical features of the [(c-Pt3)Tl(c-Pt3)]+ inorganic metallocenes. Dalton Transactions, 2013, 42, 8307. | 3.3 | 6 |
| 49 | Synthesis and Reactivity of the Unsaturated Trinuclear Phosphanido Complex [(C<sub>6</sub>F<sub>5</sub>)<sub>2</sub>Pt(Î¼-PPh<sub>2</sub>)<sub>2</sub>Pt(Î¼-PPh<sub>2</sub>)<sub>2</sub>Pt(PPh<sub>2</sub>)<sub>2</sub>]. Inorganic Chemistry, 2013, 52, 1942-1953. | 4.0 | 15 |
| 50 | Synthesis and Characterization of the Double Salts [Pt(bzq)(CNR)<sub>2</sub>][Pt(bzq)(CN)<sub>2</sub>] 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 |
| 51 | 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 |
| 52 | Binding of cerium monoxide to annulenes and buckybowls. Physical Chemistry Chemical Physics, 2012, 14, 14917. | 2.8 | 5 |
| 53 | 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 |
| 54 | Probing the electronic structure, chemical bonding, and excitation spectra of [CuE]<sup>+/0/â^'</sup> (E = 14 group element) diatomics employing DFT and ab initio methods. Journal of Computational Chemistry, 2012, 33, 2318-2331. | 3.3 | 6 |

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|---|---|---|---|
| 55 | Shedding Light on Intermolecular Metalâ€“Organic Ring Interactions by Theoretical Studies. ChemPlusChem, 2012, 77, 354-360. | 2.8 | 12 |
| 56 | 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 |
| 57 | 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 |
| 58 | Diagnosis of magnetoresponsive aromatic and antiaromatic zones in threeâ€membered rings of dâ€block and fâ€block elements. Journal of Computational Chemistry, 2010, 31, 431-446. | 3.3 | 17 |
| 59 | Structural, electronic, bonding, magnetic, and optical properties of bimetallic [Ru<sub>n</sub>Au<sub>m</sub>]<sup>0/+</sup> (n + m â‰¤ 3) clusters. Journal of Computational Chemistry, 2010, 31, 2836-2852. | 3.3 | 8 |
| 60 | 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 |
| 61 | 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 |
| 62 | One-Pot and Step-by-Step N-Assisted C<sub>Ph</sub>â^'H Activation in 2-(4-Bromophenyl)imidazol[1,2-a]pyridine: Synthesis of a New C,N-Cyclometalated Compound [{Pt(C<sup>â^§</sup>N)(Î¼-Cl)}<sub>2</sub>] as Precursor of Luminescent Platinum(II) Compounds. Organometallics, 2010, 29, 1396-1405. | 2.3 | 25 |
| 63 | 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 |
| 64 | 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 |
| 65 | 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 |
| 66 | 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 |
| 67 | 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 |
| 68 | Synthesis, characterization, DNA-binding properties and electronic structure (DFT) of ruthenium oligopyridine complexes. Inorganic Chemistry Communication, 2008, 11, 1341-1346. | 3.9 | 8 |
| 69 | 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 |
| 70 | 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 |
| 71 | 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 |
| 72 | 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 |

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| 73 | 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 |
| 74 | 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 |
| 75 | Formation of PPh2C6F5through Phosphido Platinum and/or Palladium(III) Intermediatesâ€–,âŠ¥. Organometallics, 2006, 25, 1084-1091. | 2.3 | 38 |
| 76 | 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 |
| 77 | 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 |
| 78 | 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 |
| 79 | 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 |
| 80 | All-Organometallic Analogues of Zeise's Salt for the Three Group 10 Metals. Organometallics, 2005, 24, 3539-3546. | 2.3 | 24 |
| 81 | Ligand-Stabilized Aromatic Three-Membered Gold Rings and Their Sandwichlike Complexes. Journal of the American Chemical Society, 2005, 127, 10623-10638. | 13.7 | 43 |
| 82 | 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 |
| 83 | Structure, Energetics, and Bonding of First Row Transition Metal Pentazolato Complexes:Â A DFT Study. Inorganic Chemistry, 2004, 43, 1273-1286. | 4.0 | 48 |
| 84 | 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 |
| 85 | 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 |
| 86 | 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 |
| 87 | 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 |
| 88 | 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 |
| 89 | 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 |
| 90 | 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 |

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| 91 | 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 |
| 92 | Electronic Structure and Optical Properties of Mixed Phenylene Vinylene/Phenylene Ethynylene Conjugated Oligomers. Chemistry of Materials, 2002, 14, 1362-1368. | 6.7 | 38 |
| 93 | 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 |
| 94 | 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 |
| 95 | 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 |
| 96 | 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 |
| 97 | Ab initio and density functional electronic structure study of molybdenum oxide clusters. Physical Chemistry Chemical Physics, 2000, 2, 1357-1363. | 2.8 | 18 |
| 98 | 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 |
| 99 | 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 |
| 100 | A theoretical study of molecular titanium oxide clusters: structure, bonding, vibrations and stability. Physical Chemistry Chemical Physics, 1999, 1, 4453-4458. | 2.8 | 16 |
| 101 | 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 |