# Diego CortÃ©s-Arriagada

List of Publications by Year
in descending order



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|---|---|---|---|
| 88 papers | 1,793 citations | 279701 23 h-index | 330025 37 g-index |
| 97 all docs | 97 docs citations | 97 times ranked | 1885 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Acetylsalicylic acid interaction with Boron nitride nanostructures â€“ A density functional analysis. Journal of Molecular Liquids, 2022, 355, 118980. | 2.3 | 21 |
| 2 | Chiral 1D Metalâ€“Organic Materials Based on Cu(II) and Amino Acid Schiff Bases. Crystal Growth and Design, 2022, 22, 237-250. | 1.4 | 6 |
| 3 | Tailoring the arsenic(III) removal ability from water using metal-organic frameworks via metal exchange â€“ A computational study. Journal of Molecular Liquids, 2022, 358, 119167. | 2.3 | 1 |
| 4 | A first-principles study on the adsorption properties of phosphorene oxide for pollutant removal from water. Journal of Molecular Liquids, 2022, 357, 119103. | 2.3 | 2 |
| 5 | Photophysical characteristics of Phenylimidazo(4,5-f)1,10-phenanthroline Rhenium(I) complexes - A theoretical approach to their potential applications in lighting devices. Materials Science in Semiconductor Processing, 2022, 147, 106733. | 1.9 | 0 |
| 6 | Dependence between luminescence properties of Cu(<scp>i</scp>) complexes and electronic/structural parameters derived from steric effects. New Journal of Chemistry, 2022, 46, 10584-10593. | 1.4 | 2 |
| 7 | A new CuII-dinuclear paddlewheel complex. Structural and electronic properties. Journal of Molecular Structure, 2021, 1224, 129172. | 1.8 | 5 |
| 8 | Elucidating the co-transport of bisphenol A with polyethylene terephthalate (PET) nanoplastics: A theoretical study of the adsorption mechanism. Environmental Pollution, 2021, 270, 116192. | 3.7 | 37 |
| 9 | In silico study of the adsorption of acetamiprid on functionalized carbon nanocones. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 128, 114516. | 1.3 | 11 |
| 10 | Neutral and cationic methallyl nickel complexes in alkene activation: a combined DFT, ESI-MS and chemometric approach. Catalysis Science and Technology, 2021, 11, 7475-7485. | 2.1 | 1 |
| 11 | Exploring the adsorption properties of doped phosphorene for the uptake of DNA nucleobases. Journal of Molecular Liquids, 2021, 325, 115183. | 2.3 | 6 |
| 12 | Intermolecular driving forces on the adsorption of DNA/RNA nucleobases to graphene and phosphorene: An atomistic perspective from DFT calculations. Journal of Molecular Liquids, 2021, 325, 115229. | 2.3 | 17 |
| 13 | 2-Mercaptobenzothiazole modified carbon paste electrode as a novel copper sensor: An electrochemical and computational study. Journal of Electroanalytical Chemistry, 2021, 888, 115208. | 1.9 | 13 |
| 14 | Functionalized porphyrins from meso-poly-halogeno-alkyl-dipyrromethanes: synthesis and characterization. Comptes Rendus Chimie, 2021, 24, 27-45. | 0.2 | 1 |
| 15 | First-principles study of hybrid nanostructures formed by deposited phthalocyanine/porphyrin metal complexes on phosphorene. Journal of Molecular Liquids, 2021, 333, 115948. | 2.3 | 9 |
| 16 | Enhancing the electrocatalytic activity of Fe phthalocyanines for the oxygen reduction reaction by the presence of axial ligands: Pyridine-functionalized single-walled carbon nanotubes. Electrochimica Acta, 2021, 398, 139263. | 2.6 | 27 |
| 17 | Fullereneâ€“phosphoreneâ€“nanoflake nanostructures: Modulation of their interaction mechanisms and electronic properties through the size of carbon fullerenes. Carbon, 2021, 182, 354-365. | 5.4 | 5 |
| 18 | High stability and properties of adsorbed polycyclic aromatic hydrocarbons (PAHs) onto phosphorene: An atomistic DFT study. Journal of Molecular Liquids, 2021, 341, 117465. | 2.3 | 4 |

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|---|---|---|---|
| 19 | Effective removal of water-soluble methylated arsenic contaminants with phosphorene oxide nanoflakes: A DFT study. Journal of Molecular Liquids, 2021, 341, 117423. | 2.3 | 3 |
| 20 | Removal of water-soluble inorganic arsenicals with phosphorene oxide nanoadsorbents: A first-principles study. Chemical Engineering Journal, 2021, 426, 131471. | 6.6 | 4 |
| 21 | Quantum molecular study on doping effect in titanium and vanadium clusters: their application to remove some chemical species. Applied Nanoscience (Switzerland), 2020, 10, 37-49. | 1.6 | 13 |
| 22 | Importance of the interaction adsorbent â€“adsorbate in the dyes adsorption process and DFT modeling. Journal of Molecular Structure, 2020, 1203, 127398. | 1.8 | 25 |
| 23 | Mechanistic study of the competitiveness between branched and linear polyethylene production on N-arylcyano-Î²-diketiminate nickel hydride. Polymer Chemistry, 2020, 11, 6640-6649. | 1.9 | 4 |
| 24 | Effect on the aromaticity of heterocyclic ligands by coordination with ruthenium electronâ€withdrawing metal centers. International Journal of Quantum Chemistry, 2020, 120, e26412. | 1.0 | 0 |
| 25 | Data of interaction of supported ionic liquids phases onto copper nanoparticles: A density functional theory study. Data in Brief, 2020, 33, 106562. | 0.5 | 1 |
| 26 | A first-principles description of the stability of transition-metal doped phosphorene nanosheets. Surfaces and Interfaces, 2020, 21, 100786. | 1.5 | 5 |
| 27 | Uptake of formaldehyde onto doped phosphorene nanosheets: A cluster DFT study of single and co-adsorption states. Journal of Alloys and Compounds, 2020, 831, 154885. | 2.8 | 26 |
| 28 | Studies on the solvatochromic effect and NLO response in new symmetric bimetallic Rhenium compounds. Polyhedron, 2020, 187, 114679. | 1.0 | 5 |
| 29 | Synthesis and photophysical characterization of novel Ir(III) complexes with a dipyridophenazine analogue (ppdh) as ancillary ligand. Polyhedron, 2020, 186, 114621. | 1.0 | 7 |
| 30 | Removal of arsenic from water using iron-doped phosphorene nanoadsorbents: A theoretical DFT study with solvent effects. Journal of Molecular Liquids, 2020, 307, 112958. | 2.3 | 23 |
| 31 | Exploring the Nature of Interaction and Stability between Water-Soluble Arsenic Pollutants and Metalâ€Phosphorene Hybrids: A Density Functional Theory Study. Journal of Physical Chemistry A, 2020, 124, 3662-3671. | 1.1 | 9 |
| 32 | Interaction of supported ionic liquids phases onto copper nanoparticles: A DFT study. Journal of Molecular Liquids, 2020, 310, 113089. | 2.3 | 11 |
| 33 | Highly modulated supported triazolium-based ionic liquids: direct control of the electronic environment on Cu nanoparticles. Nanoscale Advances, 2020, 2, 1325-1332. | 2.2 | 4 |
| 34 | Molecular conductance versus inductive effects of axial ligands on the electrocatalytic activity of self-assembled iron phthalocyanines: The oxygen reduction reaction. Electrochimica Acta, 2019, 327, 134996. | 2.6 | 14 |
| 35 | Impact of precipitate characteristics and precipitation conditions on the settling performance of a sulfide precipitation process: An exhaustive characterization of the aggregation behavior. Hydrometallurgy, 2019, 189, 105150. | 1.8 | 13 |
| 36 | Performance of doped graphene nanoadsorbents with first-row transition metals (Sc Zn) for the adsorption of water-soluble trivalent arsenicals: A DFT study. Journal of Molecular Liquids, 2019, 294, 111665. | 2.3 | 8 |

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| 37 | Interaction of H2O with (CuS)n, (Cu2S)n, and (ZnS)n small clusters (nâ€‰=â€‰1â€“4, 6): relation to the aggregation characteristics of metal sulfides at aqueous solutions. Journal of Molecular Modeling, 2019, 25, 291. | 0.8 | 11 |
| 38 | Chemical and Physical Viewpoints About the Bonding in Fullereneâ€“Graphene Hybrid Materials: Interaction on Pristine and Fe-Doped Graphene. Journal of Physical Chemistry C, 2019, 123, 24209-24219. | 1.5 | 13 |
| 39 | Interaction of trivalent arsenic on different topologies of Fe-doped graphene nanosheets at water environments: A computational study. Journal of Molecular Liquids, 2019, 289, 111137. | 2.3 | 16 |
| 40 | Computational quest of adsorbents based on doped graphene nanosheets for phosgene uptake, and analysis of the co-adsorption phenomena. Synthetic Metals, 2019, 252, 142-150. | 2.1 | 24 |
| 41 | Effect of Chemical Order in the Structural Stability and Physicochemical Properties of B12N12 Fullerenes. Scientific Reports, 2019, 9, 16521. | 1.6 | 39 |
| 42 | Fullerene-like boron nitride cages BxNy (xâ€‰+â€‰yâ€‰=â€‰28): stabilities and electronic properties from density functional theory computation. Journal of Molecular Modeling, 2019, 25, 21. | 0.8 | 14 |
| 43 | Substituent effects on the photophysical properties of amino-aurone-derivatives. Molecular Physics, 2019, 117, 1451-1458. | 0.8 | 6 |
| 44 | Enhancement of caffeine adsorption on boron nitride fullerene by silicon doping. Applied Nanoscience (Switzerland), 2019, 9, 317-326. | 1.6 | 15 |
| 45 | Interactions of B12N12 fullerenes on graphene and boron nitride nanosheets: A DFT study. Journal of Molecular Graphics and Modelling, 2019, 86, 27-34. | 1.3 | 62 |
| 46 | Phosphorene as a Template Material for Physisorption of DNA/RNA Nucleobases and Resembling of Base Pairs: A Cluster DFT Study and Comparisons with Graphene. Journal of Physical Chemistry C, 2018, 122, 4870-4880. | 1.5 | 55 |
| 47 | Reaction Electronic Flux Perspective on the Mechanism of the Zimmerman Di-Ï€-methane Rearrangement. Journal of Organic Chemistry, 2018, 83, 5969-5974. | 1.7 | 11 |
| 48 | Influence of the anion nature and alkyl substituents in the behavior of ionic liquids derived from phenylpyridines. Journal of Molecular Structure, 2018, 1154, 382-391. | 1.8 | 8 |
| 49 | Fe-doped graphene nanosheet as an adsorption platform of harmful gas molecules (CO, CO2, SO2 and) Tj ETQq1 1 0.784314 rgBT /O | 3.1 | 180 |
| 50 | B(C6F5)3 Promotes the catalytic activation of [N,S]-ferrocenyl nickel complexes in ethylene oligomerization. Applied Catalysis A: General, 2018, 550, 228-235. | 2.2 | 8 |
| 51 | Molecular hydrogen formation in the interstellar medium: the role of polycyclic aromatic hydrocarbons analysed by the reaction force and activation strain model. Monthly Notices of the Royal Astronomical Society, 2018, 481, 3052-3062. | 1.6 | 13 |
| 52 | Insights into the luminescent properties of anionic cyclometalated iridium(III) complexes with ligands derived from natural products. International Journal of Quantum Chemistry, 2018, 118, e25664. | 1.0 | 6 |
| 53 | Building Pyridinium Molecular Wires as Axial Ligands for Tuning the Electrocatalytic Activity of Iron Phthalocyanines for the Oxygen Reduction Reaction. ACS Catalysis, 2018, 8, 8406-8419. | 5.5 | 57 |
| 54 | Effects on the aromatic character of DNA/RNA nucleobases due to its adsorption onto graphene. International Journal of Quantum Chemistry, 2018, 118, e25699. | 1.0 | 6 |

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|---|---|---|---|
| 55 | Mechanistic details of ethylene polymerization reaction using methallyl nickel(<scp>ii</scp>) catalysts. Physical Chemistry Chemical Physics, 2018, 20, 22915-22925. | 1.3 | 5 |
| 56 | Heteroleptic Cu(<scp>i</scp>) complexes bearing methoxycarbonyl-imidoylindazole and POP ligands â€“ an experimental and theoretical study of their photophysical properties. New Journal of Chemistry, 2018, 42, 12576-12586. | 1.4 | 12 |
| 57 | Adsorption of polycyclic aromatic hydrocarbons onto graphyne: Comparisons with graphene. International Journal of Quantum Chemistry, 2017, 117, e25346. | 1.0 | 23 |
| 58 | Adsorption/desorption process of formaldehyde onto iron doped graphene: a theoretical exploration from density functional theory calculations. Physical Chemistry Chemical Physics, 2017, 19, 4179-4189. | 1.3 | 46 |
| 59 | Why Low Valent Lead(II) Hydride Complex Would be a Better Catalyst for CO<sub>2</sub> Activation than Its 14 Group Analogues?. Journal of Physical Chemistry C, 2017, 121, 12127-12135. | 1.5 | 9 |
| 60 | A DFT analysis of the adsorption of nitrogen oxides on Fe-doped graphene, and the electric field induced desorption. Applied Surface Science, 2017, 420, 446-455. | 3.1 | 65 |
| 61 | The Role of Coâ€Activation and Ligand Functionalization in Neutral Methallyl Nickel(II) Catalysts for Ethylene Oligomerization and Polymerization. Chemistry - A European Journal, 2017, 23, 10167-10176. | 1.7 | 13 |
| 62 | Oxidized and Si-doped graphene: emerging adsorbents for removal of dioxane. Physical Chemistry Chemical Physics, 2017, 19, 17587-17597. | 1.3 | 18 |
| 63 | In silico characterization of nitric oxide adsorption on a magnetic [B 24 N 36 fullerene/(TiO 2 ) 2 ] â^' nanocomposite. Applied Surface Science, 2017, 400, 283-292. | 3.1 | 32 |
| 64 | Nonlinear optical response of octupolar Zn(II) complexes incorporating highly aromatic polypyridinic ligands: Insights into the role of the metal center. Synthetic Metals, 2017, 234, 9-17. | 2.1 | 9 |
| 65 | Tailoring electroactive surfaces by non-template molecular assembly. Towards electrooxidation of L-cysteine. Electrochimica Acta, 2017, 254, 201-213. | 2.6 | 2 |
| 66 | Supramolecular Reversible Onâ€“Off Switch for Singlet Oxygen Using Cucurbit[n]uril Inclusion Complexes. Journal of Physical Chemistry C, 2017, 121, 21782-21789. | 1.5 | 29 |
| 67 | Theoretical analysis of Câ€“F bond cleavage mediated by cob[I]alamin-based structures. Journal of Molecular Modeling, 2017, 23, 264. | 0.8 | 6 |
| 68 | Fluorescence properties of aurone derivatives: an experimental and theoretical study with some preliminary biological applications. Photochemical and Photobiological Sciences, 2017, 16, 1268-1276. | 1.6 | 18 |
| 69 | New cyclometalated Ir(iii) complexes with bulky ligands with potential applications in LEC devices: experimental and theoretical studies of their photophysical properties. New Journal of Chemistry, 2016, 40, 6253-6263. | 1.4 | 13 |
| 70 | Expanding the environmental applications of metal (Al, Ti, Mn, Fe) doped graphene: adsorption and removal of 1,4-dioxane. Physical Chemistry Chemical Physics, 2016, 18, 32281-32292. | 1.3 | 23 |
| 71 | Aluminum and iron doped graphene for adsorption of methylated arsenic pollutants. Applied Surface Science, 2016, 386, 84-95. | 3.1 | 58 |
| 72 | Insights into the use of Au19Cu and Au19Pd clusters for adsorption of trivalent arsenic. Theoretical Chemistry Accounts, 2016, 135, 1. | 0.5 | 11 |

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| 73 | A theoretical investigation of the removal of methylated arsenic pollutants with silicon doped graphene. RSC Advances, 2016, 6, 28500-28511. | 1.7 | 19 |
| 74 | Synthesis of new phosphorescent imidoyl-indazol and phosphine mixed ligand Cu(<scp>i</scp>) complexes â€“ structural characterization and photophysical properties. RSC Advances, 2016, 6, 5141-5153. | 1.7 | 24 |
| 75 | The effect of pH on the adsorption of arsenic(III) and arsenic(V) at the TiO 2 anatase [1 0 1] surface. Journal of Colloid and Interface Science, 2016, 462, 252-259. | 5.0 | 111 |
| 76 | About the electronic and photophysical properties of iridium(<scp>iii</scp>)-pyrazino[2,3-f][1,10]-phenanthroline based complexes for use in electroluminescent devices. Physical Chemistry Chemical Physics, 2016, 18, 726-734. | 1.3 | 20 |
| 77 | A Family of Ir<sup>III</sup> Complexes with High Nonlinear Optical Response and Their Potential Use in Lightâ€Emitting Devices. European Journal of Inorganic Chemistry, 2015, 2015, 4946-4955. | 1.0 | 19 |
| 78 | Binding of Trivalent Arsenic onto the Tetrahedral Au<sub>20</sub> and Au<sub>19</sub>Pt Clusters: Implications in Adsorption and Sensing. Journal of Physical Chemistry A, 2015, 119, 6909-6918. | 1.1 | 26 |
| 79 | A comparative study of Ir(<scp>iii</scp>) complexes with pyrazino[2,3-f][1,10]phenanthroline and pyrazino[2,3-f][4,7]phenanthroline ligands in light-emitting electrochemical cells (LECs). Dalton Transactions, 2015, 44, 14771-14781. | 1.6 | 39 |
| 80 | Improving As(<scp>iii</scp>) adsorption on graphene based surfaces: impact of chemical doping. Physical Chemistry Chemical Physics, 2015, 17, 12056-12064. | 1.3 | 49 |
| 81 | Evaluating the hydrogen chemisorption and physisorption energies for nitrogen-containing single-walled carbon nanotubes with different chiralities: a density functional theory study. Structural Chemistry, 2014, 25, 1045-1056. | 1.0 | 12 |
| 82 | The mechanism of chemisorption of hydrogen atom on graphene: Insights from the reaction force and reaction electronic flux. Journal of Chemical Physics, 2014, 141, 134701. | 1.2 | 27 |
| 83 | Modeling the physisorption of bisphenol A on graphene and graphene oxide. Journal of Molecular Modeling, 2013, 19, 3569-3580. | 0.8 | 47 |
| 84 | Electron Transport Properties through Graphene Oxideâ€“Cobalt Phthalocyanine Complexes. Journal of Physical Chemistry C, 2013, 117, 23664-23675. | 1.5 | 22 |
| 85 | Global and local reactivity indexes applied to understand the chemistry of graphene oxide and doped graphene. Journal of Molecular Modeling, 2013, 19, 919-930. | 0.8 | 22 |
| 86 | Removal of 4â€chlorophenol using graphene, graphene oxide, and aâ€doped graphene (A = N, B): A computational study. International Journal of Quantum Chemistry, 2013, 113, 1931-1939. | 1.0 | 33 |
| 87 | Electrical Characteristics of Cobalt Phthalocyanine Complexes Adsorbed on Graphene. Journal of Physical Chemistry C, 2011, 115, 16052-16062. | 1.5 | 38 |
| 88 | A through-space charge transfer mechanism for explaining the oxidation of 2-chlorophenol on a tetrasulphonated nickel(III) phthalocyanine. Computational and Theoretical Chemistry, 2011, 963, 161-167. | 1.1 | 6 |