

# Diego Cortés-Arriagada

## List of Publications by Year in descending order

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88  
papers

1,793  
citations

318942

23  
h-index

371746

37  
g-index

97  
all docs

97  
docs citations

97  
times ranked

2105  
citing authors

#	ARTICLE	IF	CITATIONS
1	Acetylsalicylic acid interaction with Boron nitride nanostructures – A density functional analysis. <i>Journal of Molecular Liquids</i> , 2022, 355, 118980.	2.3	21
2	Chiral 1D Metal–Organic Materials Based on Cu(II) and Amino Acid Schiff Bases. <i>Crystal Growth and Design</i> , 2022, 22, 237-250.	1.4	6
3	Tailoring the arsenic(III) removal ability from water using metal-organic frameworks via metal exchange – A computational study. <i>Journal of Molecular Liquids</i> , 2022, 358, 119167.	2.3	1
4	A first-principles study on the adsorption properties of phosphorene oxide for pollutant removal from water. <i>Journal of Molecular Liquids</i> , 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. <i>Materials Science in Semiconductor Processing</i> , 2022, 147, 106733.	1.9	0
6	Dependence between luminescence properties of Cu( $\text{L}$ ) complexes and electronic/structural parameters derived from steric effects. <i>New Journal of Chemistry</i> , 2022, 46, 10584-10593.	1.4	2
7	A new CuII-dinuclear paddlewheel complex. Structural and electronic properties. <i>Journal of Molecular Structure</i> , 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. <i>Environmental Pollution</i> , 2021, 270, 116192.	3.7	37
9	In silico study of the adsorption of acetamiprid on functionalized carbon nanocones. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 128, 114516.	1.3	11
10	Neutral and cationic methallyl nickel complexes in alkene activation: a combined DFT, ESI-MS and chemometric approach. <i>Catalysis Science and Technology</i> , 2021, 11, 7475-7485.	2.1	1
11	Exploring the adsorption properties of doped phosphorene for the uptake of DNA nucleobases. <i>Journal of Molecular Liquids</i> , 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. <i>Journal of Molecular Liquids</i> , 2021, 325, 115229.	2.3	17
13	2-Mercaptobenzothiazole modified carbon paste electrode as a novel copper sensor: An electrochemical and computational study. <i>Journal of Electroanalytical Chemistry</i> , 2021, 888, 115208.	1.9	13
14	Functionalized porphyrins from meso-poly-halogeno-alkyl-dipyrromethanes: synthesis and characterization. <i>Comptes Rendus Chimie</i> , 2021, 24, 27-45.	0.2	1
15	First-principles study of hybrid nanostructures formed by deposited phthalocyanine/porphyrin metal complexes on phosphorene. <i>Journal of Molecular Liquids</i> , 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. <i>Electrochimica Acta</i> , 2021, 398, 139263.	2.6	27
17	Fullerene–phosphorene nanoflake nanostructures: Modulation of their interaction mechanisms and electronic properties through the size of carbon fullerenes. <i>Carbon</i> , 2021, 182, 354-365.	5.4	5
18	High stability and properties of adsorbed polycyclic aromatic hydrocarbons (PAHs) onto phosphorene: An atomistic DFT study. <i>Journal of Molecular Liquids</i> , 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. <i>Journal of Molecular Liquids</i> , 2021, 341, 117423.	2.3	3
20	Removal of water-soluble inorganic arsenicals with phosphorene oxide nanoadsorbents: A first-principles study. <i>Chemical Engineering Journal</i> , 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. <i>Applied Nanoscience (Switzerland)</i> , 2020, 10, 37-49.	1.6	13
22	Importance of the interaction adsorbent – adsorbate in the dyes adsorption process and DFT modeling. <i>Journal of Molecular Structure</i> , 2020, 1203, 127398.	1.8	25
23	Mechanistic study of the competitiveness between branched and linear polyethylene production on <i>N</i> -arylcyno- <i>l</i> <sup>2</sup> -diketiminato nickel hydride. <i>Polymer Chemistry</i> , 2020, 11, 6640-6649.	1.9	4
24	Effect on the aromaticity of heterocyclic ligands by coordination with ruthenium electron-withdrawing metal centers. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26412.	1.0	0
25	Data of interaction of supported ionic liquids phases onto copper nanoparticles: A density functional theory study. <i>Data in Brief</i> , 2020, 33, 106562.	0.5	1
26	A first-principles description of the stability of transition-metal doped phosphorene nanosheets. <i>Surfaces and Interfaces</i> , 2020, 21, 100786.	1.5	5
27	Uptake of formaldehyde onto doped phosphorene nanosheets: A cluster DFT study of single and co-adsorption states. <i>Journal of Alloys and Compounds</i> , 2020, 831, 154885.	2.8	26
28	Studies on the solvatochromic effect and NLO response in new symmetric bimetallic Rhenium compounds. <i>Polyhedron</i> , 2020, 187, 114679.	1.0	5
29	Synthesis and photophysical characterization of novel Ir(III) complexes with a dipyrrophenazine analogue (ppdh) as ancillary ligand. <i>Polyhedron</i> , 2020, 186, 114621.	1.0	7
30	Removal of arsenic from water using iron-doped phosphorene nanoadsorbents: A theoretical DFT study with solvent effects. <i>Journal of Molecular Liquids</i> , 2020, 307, 112958.	2.3	23
31	Exploring the Nature of Interaction and Stability between Water-Soluble Arsenic Pollutants and Metal-Phosphorene Hybrids: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3662-3671.	1.1	9
32	Interaction of supported ionic liquids phases onto copper nanoparticles: A DFT study. <i>Journal of Molecular Liquids</i> , 2020, 310, 113089.	2.3	11
33	Highly modulated supported triazolium-based ionic liquids: direct control of the electronic environment on Cu nanoparticles. <i>Nanoscale Advances</i> , 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. <i>Electrochimica Acta</i> , 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. <i>Hydrometallurgy</i> , 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. <i>Journal of Molecular Liquids</i> , 2019, 294, 111665.	2.3	8

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37	Interaction of H <sub>2</sub> O with (CuS) <sub>n</sub> , (Cu <sub>2</sub> S) <sub>n</sub> , and (ZnS) <sub>n</sub> small clusters (n = 4, 6): relation to the aggregation characteristics of metal sulfides at aqueous solutions. <i>Journal of Molecular Modeling</i> , 2019, 25, 291.	0.8	11
38	Chemical and Physical Viewpoints About the Bonding in Fullerene-Graphene Hybrid Materials: Interaction on Pristine and Fe-Doped Graphene. <i>Journal of Physical Chemistry C</i> , 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. <i>Journal of Molecular Liquids</i> , 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. <i>Synthetic Metals</i> , 2019, 252, 142-150.	2.1	24
41	Effect of Chemical Order in the Structural Stability and Physicochemical Properties of B <sub>12</sub> N <sub>12</sub> Fullerenes. <i>Scientific Reports</i> , 2019, 9, 16521.	1.6	39
42	Fullerene-like boron nitride cages B <sub>x</sub> N <sub>y</sub> (x + y = 28): stabilities and electronic properties from density functional theory computation. <i>Journal of Molecular Modeling</i> , 2019, 25, 21.	0.8	14
43	Substituent effects on the photophysical properties of amino-aurone-derivatives. <i>Molecular Physics</i> , 2019, 117, 1451-1458.	0.8	6
44	Enhancement of caffeine adsorption on boron nitride fullerene by silicon doping. <i>Applied Nanoscience (Switzerland)</i> , 2019, 9, 317-326.	1.6	15
45	Interactions of B <sub>12</sub> N <sub>12</sub> fullerenes on graphene and boron nitride nanosheets: A DFT study. <i>Journal of Molecular Graphics and Modelling</i> , 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. <i>Journal of Physical Chemistry C</i> , 2018, 122, 4870-4880.	1.5	55
47	Reaction Electronic Flux Perspective on the Mechanism of the Zimmerman Di- $\pi$ -methane Rearrangement. <i>Journal of Organic Chemistry</i> , 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. <i>Journal of Molecular Structure</i> , 2018, 1154, 382-391.	1.8	8
49	Fe-doped graphene nanosheet as an adsorption platform of harmful gas molecules (CO, CO <sub>2</sub> , SO <sub>2</sub> and Tj ETQq1 1,0,784314 rgBT / O	3.1	189
50	B(C <sub>6</sub> F <sub>5</sub> ) <sub>3</sub> Promotes the catalytic activation of [N,S]-ferrocenyl nickel complexes in ethylene oligomerization. <i>Applied Catalysis A: General</i> , 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. <i>Monthly Notices of the Royal Astronomical Society</i> , 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. <i>International Journal of Quantum Chemistry</i> , 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. <i>ACS Catalysis</i> , 2018, 8, 8406-8419.	5.5	57
54	Effects on the aromatic character of DNA/RNA nucleobases due to its adsorption onto graphene. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25699.	1.0	6

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55	Mechanistic details of ethylene polymerization reaction using methallyl nickel catalysts. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 22915-22925.	1.3	5
56	Heteroleptic Cu complexes bearing methoxycarbonyl-imidoylindazole and POP ligands: an experimental and theoretical study of their photophysical properties. <i>New Journal of Chemistry</i> , 2018, 42, 12576-12586.	1.4	12
57	Adsorption of polycyclic aromatic hydrocarbons onto graphyne: Comparisons with graphene. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25346.	1.0	23
58	Adsorption/desorption process of formaldehyde onto iron doped graphene: a theoretical exploration from density functional theory calculations. <i>Physical Chemistry Chemical Physics</i> , 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?. <i>Journal of Physical Chemistry C</i> , 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. <i>Applied Surface Science</i> , 2017, 420, 446-455.	3.1	65
61	The Role of Co-Activation and Ligand Functionalization in Neutral Methallyl Nickel(II) Catalysts for Ethylene Oligomerization and Polymerization. <i>Chemistry - A European Journal</i> , 2017, 23, 10167-10176.	1.7	13
62	Oxidized and Si-doped graphene: emerging adsorbents for removal of dioxane. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17587-17597.	1.3	18
63	In silico characterization of nitric oxide adsorption on a magnetic [B <sub>24</sub> N <sub>36</sub> fullerene/(TiO <sub>2</sub> ) <sub>2</sub> ] nanocomposite. <i>Applied Surface Science</i> , 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. <i>Synthetic Metals</i> , 2017, 234, 9-17.	2.1	9
65	Tailoring electroactive surfaces by non-template molecular assembly. Towards electrooxidation of L-cysteine. <i>Electrochimica Acta</i> , 2017, 254, 201-213.	2.6	2
66	Supramolecular Reversible On/Off Switch for Singlet Oxygen Using Cucurbit[5]uril Inclusion Complexes. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21782-21789.	1.5	29
67	Theoretical analysis of C-F bond cleavage mediated by cobalt-amin-based structures. <i>Journal of Molecular Modeling</i> , 2017, 23, 264.	0.8	6
68	Fluorescence properties of aurone derivatives: an experimental and theoretical study with some preliminary biological applications. <i>Photochemical and Photobiological Sciences</i> , 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. <i>New Journal of Chemistry</i> , 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. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32281-32292.	1.3	23
71	Aluminum and iron doped graphene for adsorption of methylated arsenic pollutants. <i>Applied Surface Science</i> , 2016, 386, 84-95.	3.1	58
72	Insights into the use of Au <sub>19</sub> Cu and Au <sub>19</sub> Pd clusters for adsorption of trivalent arsenic. <i>Theoretical Chemistry Accounts</i> , 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( <i>scpi</i> ) complexes – 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 <sub>2</sub> 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( <i>scpii</i> )-pyrazino[2,3- <i>f</i> ][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 Light-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( <i>scpii</i> ) complexes with pyrazino[2,3- <i>f</i> ][1,10]phenanthroline and pyrazino[2,3- <i>f</i> ][4,7]phenanthroline ligands in light-emitting electrochemical cells (LECs). Dalton Transactions, 2015, 44, 14771-14781.	1.6	39
80	Improving As( <i>scpii</i> ) 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 Oxide–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 4-chlorophenol using graphene, graphene oxide, and 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