

NOMBRE: DIEGO ANDRÉS CORTÉS ARRIAGADA

ESTUDIOS

ANTECEDENTES ACADÉMICOS	ÁREA DEL CONOCIMIENTO	INSTITUCIÓN	AÑO
TÍTULO PROFESIONAL	Profesor y Licenciado en Educación Química y Ciencias Naturales	Universidad Metropolitana de Ciencias de la Educación	2009
MAGÍSTER	---	---	---
DOCTORADO	Química	Universidad de Santiago de Chile	2013
POSTDOCTORADO	Química Computacional	Pontificia Universidad Católica de Chile	

ACTIVIDADES DOCENTES

NIVEL	ESPECIALIDAD	INSTITUCIÓN	AÑO
PREGRADO	Química General	Pontificia Universidad Católica de Chile	2016
PREGRADO	Laboratorio Química General	Universidad Andrés Bello	2013
PREGRADO	Taller Química General	Universidad Andrés Bello	
PREGRADO	Taller Física Moderna y Electromagnetismo	Universidad Metropolitana de Ciencias de la Educación	2006-2008
POSTGRADOS	---	---	---
DOCTORADO	Laboratorio de Química Computacional - Físicoquímica Avanzada	Pontificia Universidad Católica de Chile	2013-2016
OTROS	---	---	---

PUBLICACIONES últimos 5 años

TÍTULO	TIPO DE PUBLICACIÓN	AÑO
Importance of the interaction adsorbent – Adsorbate in the dyes adsorption process and DFT modeling	ISI	2020
Quantum molecular study on doping effect in Titanium and Vanadium clusters: Their application to remove some chemical species	ISI	2020
Effect of Chemical Order in the Structural Stability and Physicochemical Properties of B12N12 Fullerenes	ISI	2019
Molecular Conductance versus Inductive Effects from Axial Ligands on the Electrocatalytic Action for ORR of Self-Assembled Iron Phthalocyanine	ISI	2019
Chemical and Physical Viewpoints About the Bonding in Fullerene-Graphene Hybrid Materials: Interaction on Pristine and Fe-Doped Graphene	ISI	2019
Impact of precipitates on the settling performance of a sulfide precipitation process: An exhaustive characterization of the aggregation behavior	ISI	2019
Performance of doped graphene nanoadsorbents with first-row transition metals (Sc-Zn) for the adsorption of water-soluble trivalent arsenicals: A DFT Study	ISI	2019

Interaction of H ₂ O with (CuS) _n , (Cu ₂ S) _n and (ZnS) _n small clusters (n=1-4, 6): Relation to the aggregation characteristics of metal sulfides at aqueous solutions	ISI	2019
Interaction of trivalent arsenic on different topologies of Fe-doped graphene nanosheets at water environments: A computational study	ISI	2019
Computational quest of adsorbents based on doped graphene nanosheets for phosgene uptake, and analysis of the co-adsorption phenomena	ISI	2019
Interactions of B ₁₂ N ₁₂ fullerenes on graphene and boron nitride nanosheets: A DFT study	ISI	2019
Fullerene-like boron nitride cages B _x N _y (x+y=28): Stabilities and electronic properties from Density Functional Theory computation	ISI	2019
Substituent Effects on the Photophysical Properties of Amino-Aurone-Derivatives	ISI	2019
Enhancement of Caffeine Adsorption on Boron Nitride Fullerene by Silicon Doping	ISI	2019
Molecular Hydrogen Formation in the Interstellar Media: The Role of Polycyclic Aromatic Hydrocarbons analyzed by the Reaction Force and Activation Strain Model	ISI	2018
Mechanistic Details of the Ethylene Polymerization Reaction: Effect of Ligand Functionalization on Methallyl Nickel (II) Catalysts	ISI	2018
Building Pyridinium Molecular Wires as Axial Ligands for Tuning the Electrocatalytic Activity of Iron Phthalocyanines for the Oxygen Reduction Reaction	ISI	2018
Heteroleptic Cu(I) complexes bearing methoxycarbonyl-imidoylindazole and POP ligands - An experimental and theoretical study of their photophysical properties	ISI	2018
Effects on the aromatic character of DNA/RNA nucleobases due to its adsorption onto graphene	ISI	2018
Insights into the luminescent properties of anionic cyclometalated Ir(III) complexes with ligands derived from natural products	ISI	2018
Reaction Electronic Flux Perspective on the Mechanism of the Zimmerman Di-π-Methane Rearrangement	ISI	2018
Phosphorene as a template material for physisorption of DNA/RNA nucleobases and resembling of base pairs: A cluster DFT study and comparisons with graphene	ISI	2018
B(C ₆ F ₅) ₃ promotes the catalytic activation of [N,S]-ferrocenyl nickel complexes in ethylene oligomerization	ISI	2018
Influence of the anion nature and alkyl substituents in the behavior of ionic liquids derived from phenylpyridines	ISI	2018
Fe-doped Graphene Nanosheets as Adsorption Platforms of Harmful Gas Molecules (CO, CO ₂ , SO ₂ and H ₂ S), and the co-adsorption in O ₂ environments	ISI	2018
Nonlinear Optical Response of Octupolar Zn(II) Complexes Incorporating Highly Aromatic Polypyridinic Ligands: Insights into the Role of the Metal Center	ISI	2017
Supramolecular Control of Singlet Oxygen Generation Using Cucurbit[n]urils Inclusion Complexes	ISI	2017
Tailoring electroactive surfaces by non-template molecular assembly. Towards the electrooxidation of L-cysteine	ISI	2017
A theoretical analysis of the C-F bond cleavage mediated by Cobalt(II) porphyrin based structures	ISI	2017
Oxidized and Si-doped Graphene: Emerging Adsorbents for Removal of 1,4-Dioxane	ISI	2017

Fluorescence Properties of Aurone Derivatives: An Experimental and Theoretical Study with Some Preliminary Biological Applications	ISI	2017
A DFT analysis of the adsorption of nitrogen oxides on Fe-doped graphene, and the electric field induced desorption	ISI	2017
"The Role of the co-Activation and Ligand Functionalization in Neutral Methallyl Nickel (II) Catalysts for Oligomerization and Polymerization of Ethylene	ISI	2017
Why Low Valent Pb Hydride Complex Would be a Better Catalyst for CO Activation than its 14 Group Analogs?	ISI	2017
Adsorption of Polycyclic Aromatic Hydrocarbons (PAHs) onto Graphyne: Comparisons with Graphene	ISI	2017
In Silico characterization of Nitric Oxide Adsorption on a Magnetic [B24N36 Fullerene/(TiO2)2]- Nanocomposite	ISI	2017
Adsorption/Desorption process of Formaldehyde onto Iron Doped Graphene: A Theoretical Exploration from Density Functional Theory Calculations	ISI	2017
Expanding the Environmental Applications of Metal (Al, Ti, Mn, Fe) Doped Graphene: Adsorption and Removal of 1,4-Dioxane	ISI	2016
Aluminum and Iron Doped Graphene for Adsorption of Methylated Arsenic Pollutants	ISI	2016
New cyclometalated Ir(III) complexes with bulky ligands with potential applications in LEC devices. Experimental and theoretical studies of their photophysical properties	ISI	2016
Theoretical Investigation of the Removal of Methylated Arsenic Pollutants with Silicon Doped Graphene	ISI	2016
Insights into the use of Au ₁₉ Cu and Au ₁₉ Pd Clusters for Adsorption of Trivalent Arsenic	ISI	2016
Synthesis of new phosphorescent imidoyl-indazol and phosphines mixed ligand Cu(I) complexes - Structural characterization and photophysical properties	ISI	2016
The effect of pH on the adsorption of arsenic(III) and arsenic(V) at the TiO ₂ anatase [101] surface	ISI	2016
About the electronic and photophysical properties of Iridium (III)-pyrazino[2,3-f][1,10]-phenanthroline based complexes for use in electroluminescent devices	ISI	2016
A family of Ir(III) complexes with high non-linear optical response and potential use in light emitting devices	ISI	2015
Comparative study of Ir(III) complexes with pyrazino[2,3-f][1,10]phenanthroline and pyrazino[2,3-f][4,7]phenanthroline ligands in light-emitting electrochemical cells (LECs)	ISI	2015
Binding of trivalent arsenic onto the tetrahedral Au ₂₀ and Au ₁₉ Pt clusters: implications in adsorption and sensing	ISI	2015
Improving the As(III) adsorption on graphene based surfaces: impact of the chemical doping	ISI	2015
The mechanism of chemisorption of hydrogen atom on graphene: Insights from the reaction force and reaction electronic flux	ISI	2014
Evaluating the hydrogen chemisorption and physisorption energies for nitrogen-containing single-walled carbon nanotubes with different chiralities: a density functional theory study	ISI	2014

PROYECTOS DE INVESTIGACIÓN EN PROYECTOS CONCURSABLES últimos 5 años

NOMBRE	ROL	AÑO
Conicyt, Fondecyt Regular 2020. "Specific Zn(II) additives for improved Light Emitting Electrochemical Cells based on Ir(III)	Co-Investigador	2020-2023

complexes containing N-heterocyclic carbenes, with emissions at full color and white" Seleccionado para adjudicacion. Folio pendiente.		
UTEM: Concurso Interno de Fomento a la I+D+i o Creación 2018; Línea 3: Proyectos de Fortalecimiento para Equipamiento Científico y Tecnológico. L318-04 "Clúster de Computación Acelerada por GPU	Coordinador responsable	2019-2020
Conicyt, VII Concurso de Equipamiento Científico y Tecnológico Mediano FONDEQUIP, EQM180180. "Clúster Supermicro para Cómputo Científico"	Coordinador responsable	2018-2019
Conicyt, Fondecyt Iniciación en Investigación 2017, 11170289. "Theoretical characterization of the interaction of arsenic onto low-dimensional materials: Implications in adsorption of pollutants".	Investigador Responsable	2017-2020
Conicyt, Programa de Cooperación Internacional, Apoyo a la Formación de Redes Internacionales para Investigadores en Etapa Inicial, REDI170303. "Red Internacional para el estudio de sistemas híbridos Grafeno-Fulereno".	Investigador Responsable Nacional	2019-2020
Postdoctorado en Laboratorio de Química Teórica Computacional, Facultad de Química, Pontificia Universidad Católica de Chile (PUC). Proyecto Fondecyt/Postdoctorado #3140314. "Adsorción de contaminantes sobre grafeno: Estudio teórico de los modos y mecanismos de interacción, y optimización del proceso de adsorción".	Investigador Responsable	2013-2014