



CHRISTIAN ALEJANDRO CELAYA LOPEZ

Datos Generales

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Máximo nivel de estudios: LICENCIATURA

Antigüedad académica en la UNAM: 4 años

Nombramientos

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Instituto de Investigaciones en Materiales
Desde 16-01-2026

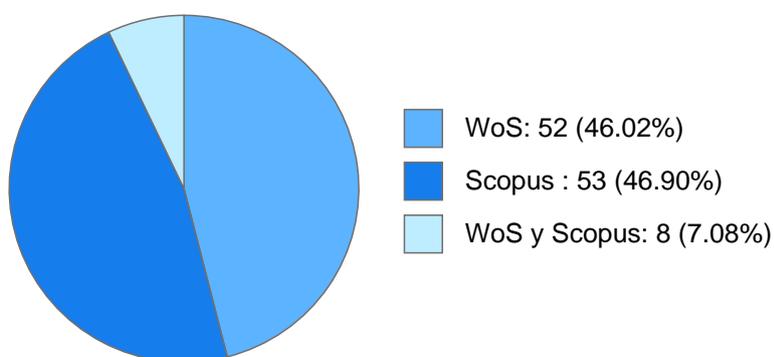
Estímulos, programas, premios y reconocimientos

SNI I 2022 - 2023

CHRISTIAN ALEJANDRO CELAYA LOPEZ

DOCUMENTOS EN REVISTAS

Histórico de Documentos



#	Título	Autores	Revista	Año
1	Understanding the enhanced thermal stability of astaxanthin loaded onto functionalized biogenic porous silica: Experimental and theoretical approach	CHRISTIAN ALEJANDRO CELAYA LOPEZ JESUS MUÑIZ SORIA Arteaga-Castrejón A.A. et al.	Surfaces And Interfaces	2026
2	The influence of electron transport at perovskite/carbon interfaces to tailor photosupercapacitor devices: A DFT approach	ANGEL MANUEL GOMEZ CORONEL CORNELIO DELESMA DIAZ CHRISTIAN ALEJANDRO CELAYA LOPEZ et al.	SOLAR ENERGY	2026
3	Exploring PtAg onto silanized biogenic silica as an electrocatalyst for H ₂ evolution: A combined experimental and theoretical investigation	NAVEEN KUMAR REDDY BOGIREDDY CHRISTIAN ALEJANDRO CELAYA LOPEZ JESUS MUÑIZ SORIA et al.	JOURNAL OF COLLOID AND INTERFACE SCIENCE	2025
4	Green synthesis of glycolic acid through the electrocatalytic reduction of oxalic acid over black TiO ₂ : An experimental and theoretical study	HUGO OLVERA VARGAS OSCAR ANDRES JARAMILLO QUINTERO CHRISTIAN ALEJANDRO CELAYA LOPEZ et al.	JOURNAL OF ENERGY CHEMISTRY	2025
5	Tailoring aqueous electrolytes based on M = Li, Na and K for the α-MnO ₂ electrode and its applications for energy storage devices: A DFT approach	CORNELIO DELESMA DIAZ CHRISTIAN ALEJANDRO CELAYA LOPEZ LUIS ENRIQUE SANSORES CUEVAS et al.	APPLIED SURFACE SCIENCE	2025

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6	Exploring contaminants and analyte adsorption on functionalized porous silicon: Insights from a combined theoretical and experimental approach	CHRISTIAN ALEJANDRO CELAYA LOPEZ ANGEL MANUEL GOMEZ CORONEL JESUS MUÑIZ SORIA et al.	Surfaces And Interfaces	2025
7	Experimental and theoretical approaches to unveil the interaction mechanisms of carbon dots with 4-nitrophenol	NAVEEN KUMAR REDDY BOGIREDDY CHRISTIAN ALEJANDRO CELAYA LOPEZ JESUS MUÑIZ SORIA et al.	JOURNAL OF HAZARDOUS MATERIALS	2025
8	Formation of polysulfides as a smart strategy to selectively detect H ₂ S in a Bi(<i>iii</i>)-based MOF material	JUAN CARLOS OBESO JUREIDINI CHRISTIAN ALEJANDRO CELAYA LOPEZ Valeria B. Lopez-Cervantes et al.	CHEMICAL SCIENCE	2025
9	(Hf)PCN-224(Co) as an efficient ppm-level sensor for toxic SO ₂	NORA SOYUKI PORTILLO VELEZ CHRISTIAN ALEJANDRO CELAYA LOPEZ DIEGO SOLIS IBARRA et al.	Materials Today Advances	2025
10	Adsorption of procarbazine anticancer drug over C ₂₄ and B ₁₂ N ₁₂ nanocages: A comparative DFT study	CHRISTIAN ALEJANDRO CELAYA LOPEZ LUIS FELIPE HERNANDEZ AYALA DIEGO DANIEL GONZALEZ ARAIZA et al.	JOURNAL OF MOLECULAR GRAPHICS & MODELLING	2025
11	Exploring electron transport at the interface of MnO ₂ /carbon nanostructures for energy storage applications: A quantum chemistry approach	CORNELIO DELESMA DIAZ CHRISTIAN ALEJANDRO CELAYA LOPEZ ANA KARINA CUENTAS GALLEGOS et al.	APPLIED SURFACE SCIENCE	2025
12	Carbon monoxide sensing materials design using catalytic oxidation on MoS ₂ decorated with (ZnO) ₁₂ bubbles	CHRISTIAN ALEJANDRO CELAYA LOPEZ ANA KARINA CUENTAS GALLEGOS LUIS ENRIQUE SANSORES CUEVAS et al.	Surfaces And Interfaces	2025
13	Synergistic effects of Bi-metal oxide/graphene oxide nanocomposites in photodegradation applications	CHRISTIAN ALEJANDRO CELAYA LOPEZ Kishore G. Pritha P. et al.	Next Nanotechnology	2025
14	Exploring the hydrogen interaction on Zn ₁₂ O ₁₂ nanocages: A first-principles study	CHRISTIAN ALEJANDRO CELAYA LOPEZ Paularokiadoss F. Jeyakumar T.C. et al.	COMPUTATIONAL AND THEORETICAL CHEMISTRY	2025
15	Understanding pseudocapacitance and the SO ₃ ²⁻ reduction mechanism on Fe ₃ O ₄ electrode surface: A combined theoretical and experimental study	CHRISTIAN ALEJANDRO CELAYA LOPEZ CORNELIO DELESMA DIAZ JAVIER ALONSO LOPEZ MEDINA et al.	ELECTROCHEMICAL ACTA	2025
16	Fluorescent Sensing of SO ₂ by MFM-300(M) Metal-Organic Frameworks: Influence of Semi-Open Metal Centres	VALERIA BELEN LOPEZ CERVANTES CHRISTIAN ALEJANDRO CELAYA LOPEZ ENRIQUE JAIME LIMA MUÑOZ et al.	Small	2025

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17	DFT on the material design and understanding for energy conversion and storage: Present state and further perspectives	CORNELIO DELESMA DIAZ CHRISTIAN ALEJANDRO CELAYA LOPEZ JESUS MUÑIZ SORIA et al.	Theoretical and Computational Chemistry	2025
18	Exploring the potential of porphyrin-based materials for organic solar cells supported on carbon: A quantum chemistry approach	CHRISTIAN ALEJANDRO CELAYA LOPEZ JESUS MUÑIZ SORIA Guillén-López A. et al.	JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY	2024
19	Unveiling the structural behavior of bimetallic AuCu/TiO ₂ catalysts in the CO oxidation: A combined in-situ spectroscopic and theoretical study	DIEGO DANIEL GONZALEZ ARAIZA CHRISTIAN ALEJANDRO CELAYA LOPEZ JESUS MUÑIZ SORIA et al.	CHEMICAL ENGINEERING JOURNAL	2024
20	Exploring enhanced CFC gas adsorption on Pt decorated graphene-modified sheets: A density functional theory investigation	CHRISTIAN ALEJANDRO CELAYA LOPEZ JESSICA OLVERA MANCILLA Paularokiadoss F. et al.	DIAMOND AND RELATED MATERIALS	2024
21	Al(III)-based MOF for tetracycline removal from water: Adsorption performance and mechanism	CHRISTIAN ALEJANDRO CELAYA LOPEZ ILICH ARGEL IBARRA ALVARADO Obeso J.L. et al.	JOURNAL OF SOLID STATE CHEMISTRY	2024
22	First principles study on the potential of functionalized porous silicon to capture adverse agents to human health: The role played by the interface interactions	CHRISTIAN ALEJANDRO CELAYA LOPEZ JESUS MUÑIZ SORIA T. G. Diaz-Rodriguez	BIOPHYSICAL CHEMISTRY	2023
23	Understanding Li interaction in TiO ₂ /graphene composites for high-performance Li-ion battery anodes: A first principles study	CHRISTIAN ALEJANDRO CELAYA LOPEZ JESUS MUÑIZ SORIA EI Hachimi A.G. et al.	PHYSICA B-CONDENSED MATTER	2023
24	Efficient Removal of Lead(II), Cadmium(II) and Zinc(II) from Aqueous Solutions by Bis[2-(1H-benzimidazol-2-yl)phenyl]disulfide, a Solid Chelating Agent	CHRISTIAN ALEJANDRO CELAYA LOPEZ MIGUEL REINA TAPIA Jesus Alberto Barron-Zambrano et al.	Chemistryselect	2023
25	Understanding the role of porosity in carbon monolayers for their use as anode material for Li-ion batteries: A first principle study	CHRISTIAN ALEJANDRO CELAYA LOPEZ ANA KARINA CUENTAS GALLEGOS JESUS MUÑIZ SORIA	APPLIED SURFACE SCIENCE	2023
26	A DFT study on structural and bonding analysis of transition-metal carbonyls [M(CO) ₄] with terminal silicon chalcogenides complexes [M(CO) ₃ SiX] (M = Ni, Pd, and Pt; X = O, S, Se, and Te)	CHRISTIAN ALEJANDRO CELAYA LOPEZ Vetri P. Paularokiadoss F. et al.	COMPUTATIONAL AND THEORETICAL CHEMISTRY	2023

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27	Understanding the electronic structure of the alkaloid in scorpion venom through drug adsorption and molecular docking studies on COVID-19 proteins	CHRISTIAN ALEJANDRO CELAYA LOPEZ Ilavarasi A.V. Paularokiadoss F. et al.	Chemical Physics Impact	2023
28	Exploring the CO ₂ photocatalytic evolution onto the CuO (110) surface: A combined theoretical and experimental study	CHRISTIAN ALEJANDRO CELAYA LOPEZ RAUL SUAREZ PARRA Castro-Ocampo O. et al.	Heliyon	2023
29	Synthesis and Characterization of a Photocatalytic Material Based on Raspberry-like SiO ₂ @TiO ₂ Nanoparticles Supported on Graphene Oxide	CHRISTIAN ALEJANDRO CELAYA LOPEZ PANDIYAN THANGARASU Rios C. et al.	Molecules	2023
30	Understanding of vibrational and thermal behavior of bio-based doped alginate@nickel cross-linked beads: A combined experimental and theoretical study	CHRISTIAN ALEJANDRO CELAYA LOPEZ MIGUEL REINA TAPIA Abdellaoui Y. et al.	JOURNAL OF MOLECULAR STRUCTURE	2022
31	Understanding hydroxyl radicals addition to CO ₂ on α -Fe ₂ O ₃ (110) surface photocatalyst for organic compounds production	CHRISTIAN ALEJANDRO CELAYA LOPEZ OSCAR ANDRES JARAMILLO QUINTERO HUGO ALBERTO LARA GARCIA et al.	Fuel	2022
32	Comparison of green bio-based cerium/alginate vs. copper/alginate beads: a study of vibrational and thermal properties using experimental and theoretical methods	CHRISTIAN ALEJANDRO CELAYA LOPEZ DIEGO DANIEL GONZALEZ ARAIZA MIGUEL REINA TAPIA et al.	JOURNAL OF MOLECULAR MODELING	2022
33	Density functional theory study of the selective oxidation of 5-Hydroxymethylfurfural (HMF) to 5-Hydroxymethyl-2-furancarboxylic acid (HMFA) on the Silver oxide surface (001)	CHRISTIAN ALEJANDRO CELAYA LOPEZ Oukhrib R. El Had M.A. et al.	Molecular Catalysis	2022
34	Exploring the CO ₂ conversion into hydrocarbons via a photocatalytic process onto M-doped titanate nanotubes (M = Ni and Cu)	CHRISTIAN ALEJANDRO CELAYA LOPEZ MELISSA MENDEZ GALVAN JORGE NOE DIAZ DE LEON HERNANDEZ et al.	Fuel	2022
35	Tailoring nanostructured materials based on γ -graphyne monolayers modified with Au heteroatoms for application in energy storage devices: A first principle study	CHRISTIAN ALEJANDRO CELAYA LOPEZ LUIS ENRIQUE SANSORES CUEVAS JESUS MUÑOZ SORIA et al.	APPLIED SURFACE SCIENCE	2022

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36	Cobalt-Ceria Catalysts for the Methanol Decomposition: Insights in the Long-Term Stability and Methanol Interaction	DIEGO DANIEL GONZALEZ ARAIZA CHRISTIAN ALEJANDRO CELAYA LOPEZ LUCIANO ANTONIO GOMEZ CORTES et al.	TOPICS IN CATALYSIS	2022
37	Exploring the Fe doped borazine system as a promising CFC adsorbent: A DFT study	MIGUEL REINA TAPIA CHRISTIAN ALEJANDRO CELAYA LOPEZ Paularokiadoss F. et al.	COMPUTATIONA L AND THEORETICAL CHEMISTRY	2022
38	The Role of Cobalt Clusters (Co-n, n = 1-5) Supported on Defective gamma-Graphyne for Efficient Hydrogen Adsorption: A First Principles Study	CHRISTIAN ALEJANDRO CELAYA LOPEZ JESUS MUÑIZ SORIA ROBERTO RENE SALCEDO PINTOS et al.	Advanced Theory and Simulations	2022
39	Adsorption of melphalan anticancer drug on C-24, B12N12, B12C6N6, B6C12N12 and B6C6N12 nanocages: A comparative DFT study	CHRISTIAN ALEJANDRO CELAYA LOPEZ LUIS FELIPE HERNANDEZ AYALA FERNANDO BUENDIA ZAMUDIO et al.	JOURNAL OF MOLECULAR LIQUIDS	2021
40	Tuning the band gap of M-doped titanate nanotubes (M = Fe, Co, Ni, and Cu): an experimental and theoretical study	MELISSA MENDEZ GALVAN CHRISTIAN ALEJANDRO CELAYA LOPEZ OSCAR ANDRES JARAMILLO QUINTERO et al.	Nanoscale Advances	2021
41	C-36 and C35E (E=N and B) Fullerenes as Potential Nanovehicles for Neuroprotective Drugs: A Comparative DFT Study	MIGUEL REINA TAPIA CHRISTIAN ALEJANDRO CELAYA LOPEZ JESUS MUÑIZ SORIA	Chemistryselec t	2021
42	Theoretical study of Au-20/WS2 composite material as a potential candidate for the capture of XO (X=C, N, S) gases	CHRISTIAN ALEJANDRO CELAYA LOPEZ MIGUEL REINA TAPIA JESUS MUÑIZ SORIA et al.	Computational Condensed Matter	2021
43	Understanding CO2 conversion into hydrocarbons via a photoreductive process supported on the Cu2O(100), (110) and (111) surface facets: A first principles study	CHRISTIAN ALEJANDRO CELAYA LOPEZ JESUS MUÑIZ SORIA Delesma C. et al.	Fuel	2021
44	Unveiling the electronic structure nature of twisted hybrid perovskites for solar cell applications: A combined experimental and theoretical study	CHRISTIAN ALEJANDRO CELAYA LOPEZ OSCAR ANDRES JARAMILLO QUINTERO JESUS MUÑIZ SORIA et al.	SOLAR ENERGY	2021
45	Molecular knot with nine crossings: Structure and electronic properties from density functional theory computation	CHRISTIAN ALEJANDRO CELAYA LOPEZ ROBERTO RENE SALCEDO PINTOS LUIS ENRIQUE SANSORES CUEVAS	JOURNAL OF MOLECULAR GRAPHICS & MODELLING	2020

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46	Exploring the potential of graphene oxide as a functional material to produce hydrocarbons via photocatalysis: Theory meets experiment	CHRISTIAN ALEJANDRO CELAYA LOPEZ PATRICIO JAVIER VALADES PELAYO OSCAR ANDRES JARAMILLO QUINTERO et al.	Fuel	2020
47	Structures, stabilities and aromatic properties of endohedrally transition metal doped boron clusters $M@B-22$, $M = Sc$ and Ti : a theoretical study	CHRISTIAN ALEJANDRO CELAYA LOPEZ FERNANDO BUENDIA ZAMUDIO ALAN JOEL MIRALRIO PINEDA et al.	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	2020
48	A method for designing a novel class of gold-containing molecules	CHRISTIAN ALEJANDRO CELAYA LOPEZ Mesias Orozco-Ic Maria Dimitrova et al.	CHEMICAL COMMUNICATIONS	2020
49	Calculation of magnetic response properties of tetrazines	CHRISTIAN ALEJANDRO CELAYA LOPEZ Mesias Orozco-Ic Dage Sundholm	RSC ADVANCES	2020
50	C_n and C_n-1B Fullerenes as Potential Nanovehicles for Piribedil Neuroprotective Drug ($n=20, 36$ and 60)	MIGUEL REINA TAPIA CHRISTIAN ALEJANDRO CELAYA LOPEZ JESUS MUÑIZ SORIA	Chemistryselect	2019
51	Theoretical study of graphyne- γ doped with N atoms: The quest for novel catalytic materials	CHRISTIAN ALEJANDRO CELAYA LOPEZ LUIS ENRIQUE SANORES CUEVAS Muñiz J.	Fuel	2019
52	Structure, stability, and electronic structure properties of quasi-fullerenes C_{n-q} ($n=42, 48$ and 60) doped with transition metal atoms ($M=Sc, Ti, V$ and Cr): A Density Functional Theory study	CHRISTIAN ALEJANDRO CELAYA LOPEZ JESUS MUÑIZ SORIA LUIS ENRIQUE SANORES CUEVAS	COMPUTATIONAL AND THEORETICAL CHEMISTRY	2019
53	Are Small Quasi-Fullerenes Capable of Encapsulating Trimetallic Nitrides A_3-xB_xN ($A, B = Sc, Y, La, x=0-3$)? A DFT Study	CHRISTIAN ALEJANDRO CELAYA LOPEZ MIGUEL REINA TAPIA JESUS MUÑIZ SORIA et al.	Chemistryselect	2018



Sistema Integral de Información Académica
Coordinación de Planeación, Evaluación y
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Reporte individual



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LIBROS Y CAPITULOS CON ISBN

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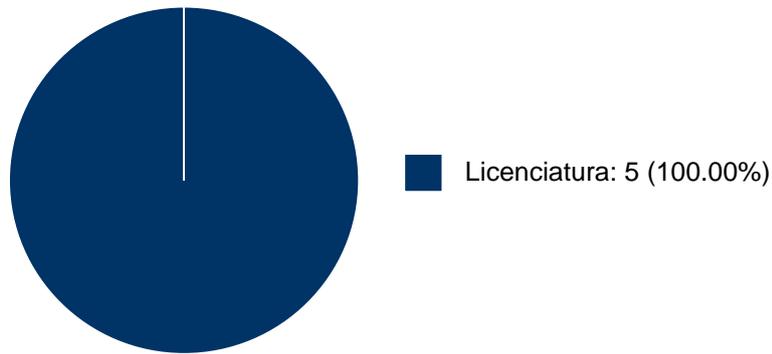
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DOCENCIA IMPARTIDA

Histórico de docencia



#	Nivel titulación	Asignatura	Entidad	Alumnos	Semestre
1	Licenciatura	CIENCIA BASICA	Facultad de Ciencias	16	2022-2
2	Licenciatura	CIENCIA BASICA	Facultad de Ciencias	13	2022-1
3	Licenciatura	CIENCIA BASICA	Facultad de Ciencias	33	2021-2
4	Licenciatura	CIENCIA BASICA	Facultad de Ciencias	11	2021-1
5	Licenciatura	CIENCIA BASICA	Facultad de Ciencias	33	2020-2



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PATENTES

No se encuentran registros en la base de datos de patentes asociados a:

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FUENTES DE INFORMACIÓN

Internos

#	Información	Fuente	Sistema	Periodo
1	Grupos ordinarios y resumen de historias académicas	DGAE	SIAE	2008-2026
2	Nombramientos, datos generales, estímulos, premios y reconocimientos	DGAPA	RUPA	2008-2026
3	Producción Académica	CH	Humanindex	2008-2021
4	Producción Académica	CIC	SCIC	2000-2017
5	Proyectos	DGPO	SISEPRO	2018-2022
6	Tesis	DGB	TESIUNAM	2008-2025
7	Tutorías en Posgrado	CGEP	SIIPosgrado	2008-2021

Externos

#	Información	Fuente	Sistema	Periodo
8	Documentos Indexados	Elsevier	Scopus	2008-2026
9	Documentos Indexados	Thomson Reuters	WoS	2008-2026
10	Obras con registro ISBN	INDAUTOR	Agencia ISBN	2008-2026
11	Patentes	IMPI	SIGA	2008-2024