

Axel Melchor Gaona Carranza

CURRICULUM VITAE

B.S. in Nanotechnology

MSc in Theoretical Chemistry and Computational Modelling

Mendoza Laboratory – Department of Chemical Engineering and Materials Science, MSU
Computational Materials Science Group – Zernike Institute for Advanced Materials, University of Groningen
Molecular Materials Theoretical Chemistry Group – ICMol, Universitat de València
Virtual Materials Modelling Laboratory – CNyN-UNAM
Email: g6_gaon17@ens.cnyn.unam.mx; Whatsapp: +52 (844) 128 2884;
Google Scholar: <https://scholar.google.com/citations?user=jkDsR9sAAAAJ>
ORCID: <https://orcid.org/0000-0001-5911-1512>

EDUCATION

M. Sc. in Theoretical Chemistry and Computational Modeling (Erasmus Mundus Program)

University of Valencia, Valencia, Spain.

Graduation date: June 2023

Bachelor of Science in Nanotechnology

Center for Nanoscience and Nanotechnology, UNAM, Ensenada, Mexico.

Graduation date: June 2021

LANGUAGES: Spanish (Native language) and English (IELTS C1 Level).

CURRENT RESEARCH:

- **Michigan State University, East Lansing, MI, United States., March 2024 – Currently**

Investigating electronic and vibrational phenomena of materials in the José Luis Mendoza's Group. Phonon calculations to investigate the impact of grain size and crystallinity of halide perovskite films, first-principles calculations of defects in $\text{WSe}_2/\text{SnSe}_2$ heterostructures and high-throughput screening of promising materials for redox stability with Machine Learning techniques to find next-generation energy materials.

GRADUATE RESEARCH:

- **Zernike Institute, University of Groningen, Groningen, Netherlands., February 2023 – June 2023**

Investigated 2D tellurium with DFT calculations of layer's stability by phonon calculations, spin-resolved electronic band structures, spin textures (2D fermi surfaces) over all the Brillouin zone, and the spin Hall effect (spin Hall tensor) through pseudo-atomic orbitals generated from DFT wavefunctions with the PAOFLOW tool for charge-to-spin conversion, under supervision of Dr. Jagoda Slawinska (Groningen) and Dr. Joaquín Calbo (València).

- **ICMol-UV, Universitat de València, València, Spain., September 2021 – June 2023**

Discussion through DFT calculations using the Quantum ESPRESSO and FHI-AIMS packages the optical measurements made by experimentalists on chalcogenide antiperovskite thin films (Ag_3SI and Ag_3SBr) published in the Chemistry of Materials Journal. DOI: <https://doi.org/10.1021/acs.chemmater.3c01349>

UNDERGRADUATE RESEARCH:

- **CIQA-CONACyT (L.A. García-Cerda and Dr. E. Mendoza-Mendoza), Saltillo, Coahuila, May 2017 – July 2017**

Synthesis of ZnO and Ag/ZnO heterostructures for photodegradation reactions of methylene blue.

- **CnyN-UNAM (Espiridión Martínez-Aguilar and Dr. Jesús María Siqueiros Beltrones), Ensenada, B.C., December 2017 – June 2018**

Investigated the photovoltaic effect in ferroelectric materials.

- **Nanoengineering Department (Dr. Shirley Meng), UCSD, San Diego, Cal., June 2018 – Aug 2018**

Fabrication of hybrid perovskite solar cells and studies of the hole transport layer (Spiro-OMeTAD).

- **Nanoengineering Department (Dr. Andrea Tao), UCSD, San Diego, Cal., June 2019 – Aug 2019**
Fabrication of plasmonic nanostructured metasurfaces (silver nanocubes over a gold surface) and studies for the detection of water organic pollutants through Surface-Enhanced Raman Spectroscopy.
- **CnyN-UNAM (Dr. Jonathan Guerrero), Ensenada, B.C., December 2020 – June 2021**
Predicting the stability and electronic structure of new alkali metal aurides through DFT calculations of phonon dispersions, electronic bandstructures, bader analysis, among others.

SCIENTIFIC PUBLICATIONS

JOURNAL PUBLICATION

- Axel Melchor Gaona Carranza, Reyes García Díaz, D. M. Hoat, Jesus M. Siqueiros, and Jonathan Guerrero-Sánchez. **Predicting the stability and electronic structure of alkali metal aurides.** *Journal of Physics: Condensed Matter*, 2022.
DOI: <https://dx.doi.org/10.1088/1361-648X/ac5d1a>
- Paz Sebastián-Luna, Nathan Rodkey, Adeem Saeed Mirza, Sigurd Mertens, Snigdha Lal, **Axel Melchor Gaona Carranza**, Joaquín Calbo, Marcello Righetto, Michele Sessolo, Laura M. Herz, Koen Vandewal, Enrique Ortí, Mónica Morales-Masis, Henk J. Bolink, and Francisco Palazon. **Chalcohalide Antiperovskite Thin Films with Visible Light Absorption and High Charge-Carrier Mobility Processed by Solvent-Free and Low-Temperature Methods.** *Chemistry of Materials*, 2023
DOI: <https://doi.org/10.1021/acs.chemmater.3c01349>
- Aungkan Sen, Liam J. Scanlon, **Axel Melchor Gaona Carranza**, Jose L. Mendoza-Cortes,*Johannes Pollanen,* Richard R. Lunt,* and William J. Gannon*. **Impact of Grain Size on Low-Temperature Carrier Phase Coherence Length in Polycrystalline Halide Perovskite Films.** *Advanced Materials Interface*, 2025
DOI: <https://doi.org/10.1002/admi.202500567>

POSTERS AND CONFERENCE PRESENTATIONS

- **A.M. Gaona-Carranza**, E. Martínez-Aguilar, and J.M. Siqueiros, “**I-V Characterization of noncentrosymmetric materials with Bulk Photovoltaic Effect**”, 31th Annual Undergraduate Research Conference (URC, UC, San Diego. Date: May 05, 2018).
- **Axel Melchor Gaona-Carranza**, Jesús Ricardo Carmona Moroyoqui, Shen Wang, William Getz, Øystein Fjeldberg, Shirley Meng. “**Fabricating Perovskite Solar Cells: Evaluating Spin-Coating Methods**”. (ENLACE 2018, Summer Research Experience, UCSD, San Diego, California.)
- **Axel Melchor Gaona-Carranza**, Jesús Ricardo Carmona Moroyoqui, Shen Wang, William Getz, Øystein Fjeldberg, Shirley Meng. “**Fabricating Perovskite Solar Cells: Evaluating Spin-Coating Methods**”. (International Conference on Nanotechnology Tec.nano 2018, Monterrey, Nuevo León, México)
- **Axel Melchor Gaona-Carranza**, Emmanuel de Jesús Rojas-Ramírez, Yuan Zeng, Matthew Creyer, Su-Wen Hsu, Andrea Tao. “**Building a nanostructured metasurface for molecule detection**”. (ENLACE 2019, Summer Research Experience, UCSD, San Diego, California.
- **Axel Melchor Gaona-Carranza**, Jonathan Guerrero Sánchez, Reyes García-Díaz, Jesús María Siqueiros Beltrones. “**Predicting the stability and electronic properties of alkali-ion metal aurides**”. (American Physical Society, March Meeting 2021, ONLINE.) URL: <https://meetings.aps.org/Meeting/MAR21/Session/H71.235>
- **Axel Melchor Gaona-Carranza**. Phonon Studies in Crystals. Michigan State University. July 2025 URL: https://mediaspace.msu.edu/media/20250708_GroupMeeting_Axel_PhononStudiesinCrystals/1_zcblfvmd

SKILLS:

Computational Mat. Science:	VASP, QUANTUM ESPRESSO, CRYSTAL23, FHI-aims, PHONOPY, Wannier90, PAOFLOW, GAUSSIAN, XcrysDen, Gamess, VESTA, PyProcar, CellMatch, V_sim, ascii-phonons, TB2J.
Programming & Software:	Bash (Linux Shell), Python, GNUplot, MATLAB, SolidWorks, OriginPro, LaTeX, Microsoft Office.
Characterization Techniques:	SEM/EDS/FIB/Cathodoluminescence Fundamentals & hands-on Experience; UV-Vis Spectroscopy; XRD; Raman Spectroscopy; TEM Fundamentals
Materials Synthesis:	Molten Salt Synthesis; Atomic Layer Deposition (ALD); Pulsed Laser Deposition; Evaporative Deposition Synthesis; Hydrothermal Synthesis; Spin-Coating deposition; Langmuir-Blodgett Deposition

HIGH PERFORMANCE COMPUTING EXPERIENCE:

Country	Name	Institution	Link
Mexico	Miztli	UNAM	http://www.lancad.mx/?p=59
Spain	Scientific Computing Center (CCC-UAM)	Autonomous University of Madrid	https://www.ccc.uam.es/
Italy	"GALILEO100" and "MARCONI"	Cineca	https://www.hpc.cineca.it/systems/hardware/galileo100/ https://www.hpc.cineca.it/systems/hardware/marconi/
Netherlands	Snellius: The National Supercomputer	SURF	https://www.surf.nl/en/services/compute/snellius-the-national-supercomputer
USA	ICER's HPC	Institute for Cyber-Enabled Research (ICER), MSU	https://icer.msu.edu/