PhD

Claudia Leticia Gomez Flores

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Biophysicist with expertise in multi-scale molecular modeling, machine learning, and protein systems. Experienced in bridging theoretical and experimental approaches through the development of user-friendly computational tools and databases.

Research Experience

Postdoc

03/2024 - 02/2025

Supervision Dr. Christopher V. Synatschke (synatschke@mpip-mainz.mpg.de) and Prof. Tristan Bereau (bereau@uni-heidelberg.de)

Max-Planck-Institute for Polymer research

- Project "**SAPs4Tissue**: *Self-assembling bioactive peptides for the biomimetic design of functional cell niches in human tissue models.*"
- Research on self-assembling peptides as intrinsically disordered peptides, investigating their structural dynamics through coarse grained simulations and functional properties.
- Implementation of machine learning algorithms for optimizing peptide sequence.
- Developed and maintained an internal peptide database, organizing and analyzing molecular data to facilitate structure-function relationship studies.

Tech tools: Python, OpenMM, Streamlit, HPC, UNIX

Teaching tasks "Theoretical Statistical Physics" at the Heidelberg University

Ph.D. thesis

05/2019 - 10/2022

Advisor Prof. Marcus Elstner (marcus.elstner@kit.edu)

Karlsruhe Institute of Technology

- "**Research Training Group 2450**: *Tailored Scale-Bridging Approaches to Computational Nanoscience.*"
- Implementation of neural network architectures to fit long-range and short-range energy interactions in protein disulfide exchange reactions for QM/MM simulations.
- Comparative analysis of energy potentials between *ab initio* and semi-empirical methods.
- Incorporation of data analysis machine learning and computational chemistry software workflows into an interactive Graphical User Interface, enhancing accessibility and usability of the computational tools for non-expert users.

Tech tools: Python, TensorFlow, CUDA, SimStack, UNIX, ORCA, DFTB+, Turbomole, Plumed, Gromacs, HPC

Teaching tasks "Physical Chemistry Laboratory for Beginners" and "Machine Learning for Chemists" at the Karlsruhe Institute for Technology

M.Sc thesis

08/2017 - 02/2019

Advisor Prof. Jose G. Sampedro Pérez (sampedro@mail.ifisica.uaslp.mx)

Universidad Autónoma de San Luis Potosí

- Performed full-atomistic MD simulations and molecular docking to identify and characterize ion and nucleotide binding sites in the N-domain of membrane H^+-ATPase from *Saccharomyces cerevisiae*
- Conducted functional and structural analysis using circular dichroism, absorbance and fluorescence spectroscopy.

Tech List: Gromacs, AutoDock, Origin

Internship

02/2018 - 10/2018

Supervision Prof. Edgar A. Cerda Méndez

Universidad Autónoma de San Luis Potosí

- Optical arrangement assembly for microcavities characterization at cryogenic temperatures.
- Reflectance, photorefectance and photoluminicennsce measurement at different microcavites on real and reciprocal space.

Tech List: Mathematica

Internship

05/2017 - 08/2017

Supervision Dr. Bernardo Yáñez-Soto

Universidad Autónoma de San Luis Potosí

- Characterization of glass surfaces by silanization and ionic coating.
- Measurement of dynamic contact angles between liquid interfaces over the characterized surfaces.

B.Sc thesis

06/2016 - 02/2017

Advisor Prof. Jose G. Sampedro Pérez (sampedro@mail.ifisica.uaslp.mx)

Universidad Autónoma de San Luis Potosí

- Expression and purification of the recombinant N-domain of the H^+-ATPase of *S.cerevisiae*.
- Steady-state fluorescence experiments for determining the position of nucleotide binding sites.

Tech List: Origin

Education

Ph.D. Natural Sciences *magna cum laude*

2019-2022

Karlsruhe Institute of Technology
Karlsruhe, Germany
Specialization: Physical Chemistry

M.Sc Interdisciplinary Sciences

2017-2019

Universidad Autónoma de San Luis Potosí
San Luis Potosí, México
Specialization: Biochemistry

B.Sc Biophysics

2013-2016

Universidad Autónoma de San Luis Potosí
San Luis Potosí, México

B.Sc Physics (Transfer to B.Sc Biophysics)

2011-2012

Universidad Nacional Autónoma de México
Ciudad de México, México

Additional Notes

Maternity Leave **12/2022-01/2024**

Publications

Published manuscripts: **Click here for Google scholar**

Electrostatic interactions contribute to the control of intramolecular thiol–disulfide isomerization in a protein.
D Maag, M Putzu, **CL Gómez-Flores** *et al*.
Physical Chemistry Chemical Physics (2021)

Accurate Free Energies for Complex Condensed-Phase Reactions Using an Artificial Neural Network Corrected DFTB/MM Methodology.
CL Gómez-Flores, D Maag, M Kansari *et al*.
Journal of Chemical Theory and Computation (2022)

Skills

Computational methods

- Quantum chemical calculations
- Full-atom molecular dynamics
- Coarse grained modelling
- Molecular Docking
- QM/MM
- Scientific GUI development
- Workflows and data analysis pipelines
- Data visualization
- High Performance Computing

Experimental methods

- Protein expression
- Protein purification
- Circular dichroism
- Fluorescence spectroscopy
- Absorbance spectroscopy
- Optical setups

Machine learning methods

- Protein language models
- Molecular descriptors (ACSF, SLATM...)
- Genetic algorithms
- Variational Autoencoders
- Regression and classification
- Data mining

Presentations

FAIR-DI European Conference on Data Intelligence 2024 *Karlsruhe (Germany)* **Oct 2024**

- Oral presentation "IN DEEP: INterdisciplinary DatabasE for Explainable Peptide prediction".

AI Tools in Science meetup at Max Planck Digital Library *Munich (Germany)* **June 2024**

- Oral presentation "AI Tools in Theoretical Biology".

Hybrid Workshop on Computer Simulation and Theory of Macromolecules *Hünfeld (Germany)* **April 2022**

- Oral presentation "Thiol Disulfide Exchange Reactions Using an Artificial Neural Network Corrected DFTB/MM Methodolo

Summer School: Machine Learning in Quantum Physics and Chemistry *Warsaw (Poland)* **Sept 2021**

- Poster presentation "Studying Disulfide Shuffling with the aid of Machine Learning".

Optical Communications Research Institute XVIII Week: Optics and its application *San Luis Potosí (México)* **May 2018**

- Best poster presentation at the Sci-comm category "How to measure the (*effective*) mass of light?"

Leiden International (Bio)Medical Students Conference *Leiden (Netherlands)* **March 2017**

- 2nd Best poster presentation "Structural and functional characterization of the H^+-ATPase of *Saccharomyces cerevisiae*"

28th International Conference on Science and Technology of Complex Fluids *San Luis Potosi (Mexico)* **June 2016**

- Oral presentation "Structural characterization of the H^+-ATPase of *Saccharomyces cerevisiae*"