DAVID CESAR MALASPINA

COMPUTATIONAL CHEMIST | JUNIOR DATA SCIENTIST
MATERIAL SCIENCE | DRUG DESIGN | DATA ANALYSIS

SKILLS

Molecular dynamics simulations all-atoms and coarse-grained. GROMACS, LAMMPS, NAMD, AMBER.

Free Energy Perturbation (FEP) methods and QSAR models.

Quantum chemistry calculations using GAUSSIAN.

Programming in Fortran and Python.

Data modeling in Python. PANDAS, SCIKIT-LEARN, PYTORCH.

Versioning with GITHUB and GITLAB and software management with JIRA.

English (fluent) – Spanish (native)

EXPERIENCE

APPLICATION SCIENTIST • CRESSET SOFTWARE & DISCOVERY (CAMBRIDGE, UK) • 2023
Customer training and development of case studies using Cresset Software for drug discovery. Providing training and support in Structure Based Drug Design and Ligand Based Drug Design, FEP, MD and QSAR.

MOLECULAR MODELER • RHEOCUBE – ELECTRIC ANT LAB (AMSTERDAM, NETHERLANDS)• 2022
Molecular modeling of coarse-grained systems. I worked in coding the implementation of Martini Force Field into RHEOCUBE software.

POSTDOCTORAL FELLOW • UNIVERSITAT ROVIRA I VIRGILI (TARRAGONA, SPAIN) • 2020 – 2022 (PROF. BONET AVALOS)
Molecular modeling of heat transport. I developed an internal code for Dissipative Particle Dynamics with energy conservation (DPDE) in Fortran, parallelized with OpenMP. I also performed heat transport coefficient evaluations within this framework.

MARIE-SKLODOWSKA-CURIE POSTDOCTORAL FELLOW • ICMAB-CSIC (BARCELONA, SPAIN)• 2017 – 2020 (PROF. FARAUDO)
Molecular modeling of bio-nano-interfaces. I developed models of protein corona formation, coarse-grained models of surfactants, cellulose wetting simulations, fluorinated fullerene adsorption, metal-carborane self-assembly and SARS-CoV-2 spike protein adsorption simulations.

POSTDOCTORAL FELLOW • NORTHWESTERN UNIVERSITY (EVANSTON, USA) • 2011 – 2017 (PROF. SZLEIFER)
Molecular modeling in the Biomedical Engineering Department. I worked on simulations of water models, designed a drug delivery system, studied antibody-mucin-HIV interactions, antibody conjugated nanoparticles simulations and collagen mechanical properties simulations.

https://dmalaspina.github.io/ https://www.linkedin.com/in/davidcesarmalaspina/ dmalaspina@gmail.com

DAVID CESAR MALASPINA

Computational Chemist | Junior Data Scientist
Material Science | Drug Design | Data Analysis

LATEST CONFERENCES

- Membranes in health and disease (2019-UK). "Cobalt bisdicarbollide interaction with membranes". Malaspina DC, Faraudo J.
- European Colloid and Interface Society (ECIS) meeting (2018-Slovenia). "Nano-scale roughness and hydrophobicity: the case of cellulose nano-crystals". Malaspina DC, J Faraudo.
- World Congress of Biomechanics (WCB) (2018-Ireland). "Collagen fibril mechanics under simulated enzymatic degradation". Malaspina DC, Szleifer I, Dhaher Y.

EDUCATION

CHEMICAL ENGINEER • 2008 • UNIVERSIDAD NACIONAL DEL SUR (ARGENTINA)

PHD IN MATERIAL SCIENCE • 2011 • UNIVERSIDAD NACIONAL DEL SUR (ARGENTINA)

AUTHOR OVERVIEW

28 publications in peer reviewed journals, h-index=17, 594 citations. Google scholar: https://scholar.google.com/citations?hl=es&user=Hd__uxUAAAAJ&view_op=list_works

SELECTED PUBLICATIONS

1. *"Computer Simulations of the interaction between SARS-CoV-2 spike glycoprotein and different surfaces"* DC Malaspina and J Faraudo. **Biointerphases 15, 051008 (2020)**. https://doi.org/10.1116/6.0000502

2. *"Atomistic simulations of COSAN: amphiphiles without a Head-and-Tail design have a"head and tail" surfactant behavior" DC Malaspina, C Viñas, F Teixidor, J Faraudo.* **Angewandte Chemie, 59, 8, 3088-3092 (2020). https://doi.org/10.1002/anie.201913257**

3. *"Molecular insight into the wetting behavior and amphiphilic character of cellulose nanocrystals"* DC Malaspina, J Faraudo **Advances in colloid and interface science, Volume 267, Pages 15-25 (2019). https://doi.org/10.1016/j.cis.2019.02.003**

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