DAVID CESAR MALASPINA

SENIOR MOLECULAR MODELER | JUNIOR DATA SCIENTIST

OVERVIEW

I work in molecular modeling and in data analysis.

SKILLS

Programming in Fortran and Python.

Versioning with GITHUB and GITLAB and software management with JIRA.

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

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

Quantum electronic density calculations using DFT. GAUSSIAN, GAMESS.

Finite elements calculations. COMSOL

English (fluent) – Spanish (native)

EXPERIENCE

POSTDOCTORAL FELLOW • NORTHWESTERN UNIVERSITY (EVANSTON, USA) • 2011 -- 2017
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.

MARIE-SKLODOWSKA-CURIE POSTDOCTORAL FELLOW • ICMAB-CSIC (BARCELONA, SPAIN)• 2017 – 2020
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 • UNIVERSITAT ROVIRA I VIRGILI (TARRAGONA, SPAIN) • 2020 – 2022
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.

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

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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**