DAVID CESAR MALASPINA

SENIOR COMPUTATIONAL CHEMIST | JUNIOR DATA SCIENTIST

OVERVIEW

I work in molecular modeling and simulations and in data analysis.

SKILLS

Programming in Fortran, Python and C++.

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

Metropolis Monte Carlo algorithms.

Fluent in English and native in Spanish

EXPERIENCE

POSTDOCTORAL FELLOW • NORTHWESTERN UNIVERSITY (USA) • 2011 – 2017
Molecular modeling in Biomedical Engineering Department under the direction of Prof. Igal Szleifer and Prof. Marcelo Carignano. I worked on simulations of water models, design of a drug delivery system, studied antibody-mucin-HIV interactions, antibody conjugated nanoparticles and collagen mechanical properties.

MSCA POSTDOCTORAL FELLOW • ICMAB-CSIC (SPAIN)• 2017 – 2020
Molecular modeling in for biomaterials under the direction of Prof. Jordi Faraudo. I worked on simulations of protein corona formation, coarse-grained model of a surfactant, cellulose wetting, fluorinated fullerene adsorption, metal-carborane self-assembly and SARS-CoV-2 spike protein adsorption.

POSTDOCTORAL FELLOW • UNIVERSITAT ROVIRA I VIRGILI (SPAIN) • 2020 – NOW
Molecular modeling in for biomaterials under the direction of Prof. Jordi Faraudo. I worked on simulations of protein corona formation, coarse-grained model of a surfactant, cellulose wetting, fluorinated fullerene adsorption, metalcarborane self-assembly and SARS-CoV-2 spike protein adsorption.

EDUCATION

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

PHD IN MATERIAL SCIENCE • 2011 • UNIVERSIDAD NACIONAL DEL SUR (ARGENTINA)
Thesis in structure and dynamics of supercooled water

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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.
- American Chemical Society (ACS) National Meeting (2018-USA). "Molecular dynamics study of human serum albumin protein corona in an inorganic nanoparticle". Malaspina DC, Faraudo J.

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
ORCID: 0000-0002-5420-9534

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**

4. *"Protein-surface interactions at the nanoscale: Atomistic simulations with implicit solvent models"* DC Malaspina, L Pérez-Fuentes, C Drummond, D Bastos-González et al. **Current Opinion in Colloid & Interface Science, Volume 41, Pages 40-49 (2019).** **https://doi.org/10.1016/j.cocis.2018.11.005**

5. *"Mechanical properties of a collagen fibril under simulated degradation"* DC Malaspina, I Szleifer, Y Dhaher **Journal of the mechanical behavior of biomedical materials, 75, 549-557 (2017).** **https://doi.org/10.1016/j.jmbbm.2017.08.020**

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