



UNIVERSIDADE
NOVA
DE LISBOA

MARIE SKŁODOWSKA-CURIE INDIVIDUAL FELLOWSHIPS 2018
EXPRESSION OF INTEREST FOR HOSTING MARIE CURIE FELLOWS

HOST INSTITUTION

Instituto de Tecnologia Química e Biológica António Xavier (ITQB-NOVA) | MOSTMICRO Research Unit

RESEARCH GROUP AND URL

Multiscale Modeling Lab
<http://www.itqb.unl.pt/labs/multiscale-modeling>

SUPERVISOR (NAME AND E-MAIL)

Manuel N. Melo
m.n.melo@itqb.unl.pt

SHORT CV OF THE SUPERVISOR

Manuel Melo is the head of the Multiscale Modeling lab within the MOSTMICRO unit of ITQB NOVA. The work is centered on elucidating the molecular-level details of lipid–lipid, lipid–protein, and protein–protein interactions, using coarse-grained, atomistic, and hybrid molecular dynamic simulations. Recent collaborations also focus on modeling the Gram-positive peptidoglycan. Additionally, I actively develop simulation and analysis software, with emphasis on large-scale parallelization.

Manuel Melo carried out postdoctoral work at the Marrink lab, at the University of Groningen, where he became involved in the development and application of the Martini coarse-grain model. He pursued a Ph.D. on the molecular level interactions of antimicrobial peptides with cellular membranes, using spectroscopic techniques coupled to mathematical modeling, connecting biophysics to microbiology.

5 SELECTED PUBLICATIONS

- M. N. Melo, R. Ferre and M. A. R. B. Castanho, Antimicrobial peptides: linking partition, activity and high membrane-bound concentrations; *Nature Reviews Microbiology*, 2009, 7:245-50.
- M. N. Melo, C. Arnarez, H. Sikkema, N. Kumar, M. Walko, H. J. C. Berendsen, A. Kocer, S. J. Marrink, and H. I. Ingólfsson, High-throughput simulations reveal membrane-mediated effects of alcohols on MscL gating; *Journal of the American Chemical Society* 2017, 39(7): 2664-71.
- H. I. Ingólfsson, M. N. Melo, F. J. van Eerden, C. Arnarez, C. A. Lopez, T. A. Wassenaar, X. Periole, A. H. De Vries, D. P. Tieleman and S. J. Marrink, Lipid organization of the plasma membrane; *Journal of the American Chemical Society* 2014, 136(41):14554-59.
- F. J. van Eerden, M. N. Melo, P. Frederix, X. Periole, and S. J. Marrink, Exchange Pathways of Plastoquinone and Plastoquinol in the Photosystem II Complex; *Nature Communications* 2017, 8:15214.



- J. Su, A. S. Thomas, T. Grubietz, C. Landgraf, R. Volkmer, S. J. Marrink, C. Williams and M. N. Melo, The N-terminal amphipathic helix of Pex11p self-interacts to induce membrane remodelling during peroxisome fission; BBA–Biomembranes 2018, 1860(6): 1292-300.

PROJECT TITLE AND DESCRIPTION

Multiscale simulations of the Gram-positive membrane and peptidoglycan: towards a comprehensive model of the cell wall.

The project will focus on the modeling of the bacterial membrane and cell wall. It will involve simulating cell wall components at different resolution scales -- from quantum mechanical to coarse grain molecular dynamics. Experimental collaborations are in place to validate the findings of the work. Proponents should have either a) experience with computing environments -- namely, the Linux OS and scripting languages (Python) -- or b) be keen on receiving training in this field.

SCIENTIFIC AREA WHERE THE PROJECT FITS BEST

Chemistry (CHE)