MARIE SKŁODOWSKA-CURIE POSTDOCTORAL FELLOWSHIPS 2024

EXPRESSION OF INTEREST FOR HOSTING MARIE CURIE FELLOWS

HOST INSTITUTION

NOVA School of Science and Technology - LAQV REQUIMTE

RESEARCH GROUP AND URL

CO_2 Conversion and Utilization/Bio(chemical) Process Engineering/Chemoinformatics

https://www.dq.fct.unl.pt/en/staff/researchers/goncalo-valente-da-silva-marino-carrera

SUPERVISOR (NAME AND E-MAIL)

Dr. Gonçalo Carrera, goncalo.carrera@fct.unl.pt

SHORT CV OF THE SUPERVISOR

Gonçalo Valente da Silva Mariño Carrera initiated his Researcher career as PhD student, just after completion of the Degree in Applied Chemistry, 17/(20), being awarded as second best student of that course (2003/2004) with a teaching grant. The PhD profile involves the complementary use of Machine-Learning (ML) and New Codification approaches in order to predict the reactivity profile of organic reactions and the melting point of ionic liquids (ILs). New room-temperature ILs were synthesized in the lab based on ML model predictions. The Degree internship plus PhD work resulted in eight peer-review articles, two oral and seven poster communications. The PhD was completed in 2009 with the final classification of *Aprovado por Unanimidade*. The first stage of the postdoctoral activity, 2009-2011, comprises an ERA-CHEM project grant based on the reaction of CO_2 incorporation into Glycerol, in the context of an experimental-phase behaviour/thermodynamic perspective. NOVA University, Université de Burgogne and Technische Universitat Dortmund cooperated on that project. Part of the work-plan was carried out in France and Germany. The second stage, 2011-2017, corresponds to an individual postdoctoral grant on biomolecule-based CO_2 capture frameworks and phase behaviour studies. The present stage is centred on the use of ML and new/adapted forms of codification in order to obtain predictive and interpretable models applied on physico-chemical and phase-behaviour profiles. This researcher publication score comprises 33 indexed Web-of-Science (WoS) items, including 28 peer-review articles, 3 Faraday Discussions's papers and 2 book chapters. It's consired, in addition, 1 cover feature, 1 Scopus-indexed conference article, 5 conference proceedings and 1 book chapter. The publication's impact includes 1 Nature, 2 Nature series, 1 Wikipedia, 2 JACS and 8 Chemical Review's citations. Six of this researcher's publications are available in NASA/Harvard repository. The participation/contribution with 17 selected oral communications is highlighted, including the participations in 1 Faraday Discussions, 2 EuCheMS Chemical Conferences, a COIL with additional participation as chair. The participation/contribution in 2 invited oral communications, with 1 plenary speaker/chair participation emphasized. It's highlighted an FCT/MCTES project, 2018-2021, awarded, as principal investigator, with 228641.57 euros with A classification. The mentoring activity comprises practical classes of two courses and supervision of two Msc-holder and three PhD-holder collaborators in project context, with the additional supervision of two students. The incorporation into Frontiers in Chemistry, as Review Editor, and science communication, extends the research activity. It's accounted 773/573(in 508 articles) citations and h-index 16/15 (Google Scholar/WoS). Check ORCID record for complete information: https://orcid.org/0000-0001-6978-3603.

5 SELECTED PUBLICATIONS

- G. V. S. M. Carrera*, The melting point profile of organic molecules: A Chemoinformatic approach, *Adv. Theory Simul.*, 2022, 5, 2200503. https://doi.org/10.1002/adts.202200503.
- G. V. S. M. Carrera*, J. Inês, C. E. S. Bernardes, K. Klimenko, K. Shimizu, José N. Canongia Lopes, The Solubility of Gases in Ionic Liquids: A Chemoinformatic Predictive and Interpretable Approach, *ChemPhysChem*, 2021, 22, 1-12. https://doi.org/10.1002/cphc.202100632.
- G. V. S. M Carrera*, M. Nunes da Ponte, L. P. N. Rebelo, Chemoinformatic approaches to predict the viscosities of ionic liquids and ionic liquid-containing systems. *ChemPhysChem*, 2019, 20, 2767-2773, (Cover Feature). https://doi.org/10.1002/cphc.201900593.

- G. V. S. M. Carrera, S. Gupta, J. Aires-de-Sousa, Machine learning of chemical reactivity from databases of organic reactions, *J. Comput. Aided Mol. Des.*, 2009, 23, 419-429. https://doi.org/10.1007/s10822-009-9275-2.
- G. Carrera, J. Aires-de-Sousa, Estimation of melting points of pyridinium bromides ionic liquids with decision trees and neural networks, *Green Chem.*, 2005, 7(1), 20-27. https://doi.org/10.1039/B408967G.

PROJECT TITLE AND SHORT DESCRIPTION

Structure/Property Insights Based on New Codification and Machine-Learning Approaches:

The impressive developments of Artificial Intelligence (AI) paved the way for the build-up of efficient models in different fields of knowledge. This AI concept is centred on Machine-Learning (ML) with examples, in order to find a pattern involving the numeric accessible characteristics of a given system and the property/activity of interest. The availability of examples requires extensive/curated databases (Big Data). The necessary algorithm and the adjusted codification approach complete this triad of elements. The resultant model ideally combines predictive and interpretable characteristics. The study of chemical systems, either pure compounds or even mixtures of different chemicals, comprise the field of Chemoinformatics. [1] Most of these approaches are either highly predictive and poorly interpretable or the reverse. Preliminary results on the solubility of gases in ILs [2] and melting points of organic molecules, highlights the real possibility of combining the best of two worlds in a straightforward form. [3] The current proposal combines the use of advanced algorithms and new forms of codification in order to accurately predict physico-chemical properties and simultaneously find the structural configuration responsible for a given property-profile.

[1] T. Engel, J. Gasteiger, Chemoinformatics: Basic Concepts and Methods, Wiley-VCH, Weinheim, 2018.
[2] G. V. S. M. Carrera*, J. Inês, C. E. S. Bernardes, K. Klimenko, K. Shimizu, José N. Canongia Lopes, The Solubility of Gases in Ionic Liquids: A Chemoinformatic Predictive and Interpretable Approach, *ChemPhysChem*, 2021, 22, 1-12.
[3] G. V. S. M. Carrera*, The melting point profile of organic molecules: A Chemoinformatic approach, *Adv. Theory Simul.*, 2022, 5, 2200503.

SCIENTIFIC AREA WHERE THE PROJECT FITS BEST*

CHE/ENG

***Scientific Area where the project fits best** – Please select/indicate the scientific area according to the panel evaluation areas: Chemistry (CHE) • Social Sciences and Humanities (SOC) • Economic Sciences (ECO) • Information Science and Engineering (ENG) • Environment and Geosciences (ENV) • Life Sciences (LIF) • Mathematics (MAT) • Physics (PHY)