

# Sousa Javannikkhah



Technology Centre: PMTC

Academic Mentor Dr. Matthias Vandichel

Company Partner: Sanofi Genzyme

Company Mentor: Dr. Dikshitkumar Khamar

Dr. Javannikkhah has completed his PhD (2015) in Chemical engineering at Iran University of Science and Technology (Iran), MSc (2008) in Polymer Engineering at Sharif University of Technology, and a BSc (2005) in Chemical engineering at Shiraz University Iran. Dr. Javannikkhah worked as a Lecturer and researcher at Faculty of Engineering, Azad University of Bushehr (Iran) (2012-2013), at Azad University, Science and Research Branch, (Tehran, Iran) (2016-2017) and at Iran University Science and Technology (2015-2018). In that period, she led the projects in the fields of drug delivery (both in atomistic and coarse-grained levels), polymer solutions, polymeric membrane (both atomistic and coarse-grained levels),graphdiyne-based hydrogen storage system, and graphene-based CO2 capturing system. She conducted various research projects as a Postdoctoral researcher at Aalto University (Finland) (2018-2020). More specifically at Aalto University, she has been working on

#### Dr. Matthias Vandichel

Dr. Matthias is head of the Materials and Catalysis Modelling group (<a href="https://MACATAMO-group.com">https://MACATAMO-group.com</a>). He (Mentor, Chemical Engineering, University of Limerick) is currently a lecturer of Chemical Engineering with > 9 years of experience in computational catalysis, molecular modelling, and chemical reaction engineering. Dr. Vandichel has obtained over €1M in funding, with a total value of > €5M in projects in which he has participated. He is currently mentor of 2 Marie Curie Fellows (PROCESS COFUND, Career FIT-PLUS), one postdoctoral researcher, and main supervisor of 5 PhD students working on a wide variety of topics. He is a Fellow of the Royal Society of Chemistry and Member of the Institution of Chemical Engineers. He has coauthored >55 publications, cited >3500 times (h-index = 27, Google Scholar).

#### Dr. Dikshitkumar Khamar

Dr. Dikshitkumar Khamar is Manufacturing Sciences Manager at Sanofi Waterford. He has over 15 years of research experience, of which 13 directly in pharmaceutical research, development, and manufacturing activities. He is managing the development and tech transfer-related activities for parenteral biologics and has expertise in freeze-drying, product-process characterization, and fill finish operations. His primary degree is in Pharmacy (B. Pharm), MSc in Pharmaceutical analysis, and PhD in crystallization of pharmaceuticals and he holds Six Sigma Black Belt (ASQ), and has a proven track record of application of LSS tools to improve quality and efficiency aspects in pharmaceutical productions. Furthermore, he has extensive mentoring experience; at present, he is mentoring 1 PhD student (WIT-Sanofi), 1 MSc by research (UCC-Sanofi), 1 postdoc (SSPC-Sanofi) and previously he mentored >2 PhD students and 6 research internship in Sanofi in last 4 years. Currently, he is managing a team of 15 development scientists directly including 7 PhDs. Dr. Dikshitkumar Khamar has published about ~15 papers (h-index = 9). He is currently collaborating with the SFI centre for pharmaceuticals based in UL (1 postdoc), University College Cork (1 MSc by research), Waterford Institute of Technology (1 PhD).

### Pharmaceutical Manufacturing Technology Centre (PMTC)

Situated within the Bernal Institute at the University of Limerick, PMTC is hosted in a world-class facility comprised of an experienced research team of senior and postdoctoral level researchers with extensive R&D and direct industry experience. PMTC is governed by a Centre Steering Committee (CSC), which meets on a quarterly basis. Funded by Enterprise Ireland in partnership with IDA Ireland PMTC is part of a network of Technology Centers nationally, each running industry-led research and innovation programmes.

### Sanofi Genzyme

Sanofi is the largest manufacturer of injectables worldwide, and there are numbers of research groups actively working on finding alternative ways to stabilize proteins. We currently have multiple platforms for drug products - lyophilized vials, pre-filled syringes-oral drug products. The site is working with number of research sites, focused formulation groups and looking at ways to convert existing drug products in oral delivery. Dr. Javannikkhah will get access to the large Sanofi network. Furthermore, she will be provided with complex and relevant protein modalities for research and help in the generational of experimental data to benchmark the modelling studies through access to Sanofi's state-of-the-art labs. Being embedded within Sanofi during a 3 months internship as part of the Marie Curie Career FIT-PLUS action, Sousa will also gain access and outreach to a team of scientists on site and in the global Sanofi network.

#### Host Institution - University of Limerick (UL)

With strong links to business and industry, UL excels at translational research which aims to accelerate the practical application of academic research to benefit society. UL houses some of the most innovative and successful research centers in Ireland. The Nexus Innovation Centre is a growing community of international researchers and entrepreneurs which supports new businesses and the creation of jobs. The UL campus is also central to the UL Enterprise Corridor which hosts leading R&D companies such as Johnson & Johnson.

## Sousa's project

# "Enabling drug delivery through the use of multiscale modelling and deep learning technologies"

Protein-based therapy has become a central research topic in the field of biomacromolecular medicine. However, these medicines are mostly available as injectables and strategies need to be developed make these proteins orally deliverable. In particular, the stability of proteins following oral administration is poor because of the highly acidic environment in the stomach and the short protein half-life time. Therefore, designing a protein delivery system that can protect and improve the protein's pharmaceutical effects is crucial.

Zwitterions or polyzwitterions ((poly)zwitterion) are potentially ideal materials for protein delivery due to their ability to form dense shell of cation/anion to protect proteins. The main aim is identifying effective protein delivery solutions based on zwitterions, which requires encapsulation into particles with controllable size. The (poly)zwitterions can form both micelles and vesicles, and when properly designed they can be transport platforms for hydrophobic as well as hydrophilic proteins. In this

proposal, (poly)zwitterion-based delivery systems will be designed for glucagon, with high stability and load efficiency. To achieve this goal, this project proposes development and implementation of integrated, multi-scale modelling techniques especially suited to screen different (poly)zwitterionic carriers for this specific protein under experimentally relevant conditions. Modulation of the targeted micelle or vesicle characteristics could be achieved by molecular engineering of the (poly)zwitterion. During the secondment at company partner Sanofi, the experimental this proposal will be developed and executed, i.e. the synthesis and characterization of protein-containing (poly)zwitterion vesicles. Besides extensive training opportunities in Sanofi, there are specific trainings foreseen in host lab (ab initio calculations, parameter variations, ANN construction, etc.), in universities UL (Limerick, Ireland), NTUA (Athens, Greece) and KIT (Karlsruhe, Germany). This project is a market-focused and addresses the manufacturing of innovative Active Pharmaceutical Ingredient (API) drug delivery platforms and drug release, in line with the major domain areas of the Pharmaceutical Manufacturing Technology Centre (PMTC) based in the University of Limerick. When this approach is successful, the impact for society and pharmaceutical industry will be huge.