**Webinar of 16th of May, 9h00 – 10h00 GMT**

**Professor Tao Chen (University of Surrey, UK): In-silico modelling of chemical transfer across the skin**

**Bio:** Tao Chen is a Professor of Chemical Engineering at the School of Chemistry & Chemical Engineering, University of Surrey. He received the BEng (2000) and MEng (2002) degrees both from the Department of Automation, Tsinghua University, China, and PhD (Chemical Engineering) from Newcastle University in 2006, UK. Prior to joining Surrey in 2011 he had worked as Research Associate at Newcastle University (2006-2007), then Assistant Professor at Nanyang Technological University, Singapore (2008-2010). Professor Chen’s research expertise is in computer modelling and artificial intelligence for improving product design and process efficiency in the broad chemical industry. He has provided R&D consultancy to leading organisations in the cosmetic, consumer goods and steelmaking sectors. He leads a research group of 8 PhD and postdoctoral researchers with accumulative research funding >£8m (>£2m as principal investigator). He has published 150 refereed journal articles.

**Abstract:** In this talk I will give an overview of mechanism-based, computer (in-silico) modelling methods for predicting the transfer of chemicals across the skin. As the skin is an important physical and biological barrier, this topic underpins topical and transdermal delivery, personal care and cosmetics, as well as extraction of biomarkers from the skin. I will focus on approaches that translate the fundamental chemical transfer problems into mathematical equations, the solution of which provide the prediction of the extent and kinetics of chemical transfer, as well as how it is affected by the active ingredient’s physical & chemical properties, skin biophysics, the product formulation, and external forces. I will conclude the talk with discussion of the challenges and future opportunities.

**Dr Roman Bauer (University of Surrey, UK): Agent-based computational modelling of biological tissue dynamics**

**Bio:** Dr Roman Bauer is a Senior Lecturer (Associate Professor) and Head of the Nature Inspired Computing and Engineering research group, in the Computer Science Research Centre at the University of Surrey (UK). Dr Roman Bauer received his Bachelor's and Master's Degree in Computational Science and Engineering from ETH Zuerich, Switzerland. Afterwards, he did his PhD at the Institute for Neuroinformatics (ETH Zürich/Uni Zürich). His research focuses on the computational modelling and analysis of biological dynamics, in particular those of the brain. His highly interdisciplinary research involves modern computing approaches, biological expertise, innovative machine learning methods and IT- related collaboration. Dr Bauer is co-founder and spokesperson of the international BioDynaMo collaboration, which has created the open-source and high-performance agent-based modelling software BioDynaMo ([www.biodynamo.org](http://www.biodynamo.org/)). He has published >50 peer-reviewed articles and leads the COMBYNE lab ([www.combynelab.com](http://www.combynelab.com/)) that has 10 members.

**Abstract:** Computational models of biological tissues are usually inherently complex due to the involvement of many different spatial and temporal scales. One widely used approach that addresses this issue is agent-based modelling (ABM). In ABM, individual cellular elements are modelled and simulated as autonomous entitites or “agents” that can communicate only with their immediate local neighbourhood. In this way, biological as well as physical processes are simulated, allowing the modeller to study their interactions. I will elaborate on the theoretical underpinnings of ABM, the state of the art and relevant tools. Along those lines, I’ll give an overview of the BioDynaMo software, its capabilities and example applications. Finally, I will reflect on ongoing developments and opportunities with regards to standardisation in ABM.