Hamburg University of Technology (TUHH)
Institute of Thermal Separation Processes -V8-
Eissendorfer Str. 38, DE-21073 Hamburg

Please fill out the form with the corresponding data for your abstract and send it to: aerogelconference@tuhh.de

In the E-mail you may include other files (e.g. Word, PDF or images).

Abstract Formulary

Presentation type: **Oral** ✔ **Poster** ☐

Title: Understanding Carbon Nanotube - Silica Aerogel composites from molecular simulation

Authors: Pedro Maximiano, Pedro N. Simões

Presenting author: Pedro Maximiano

Institution (Presenter): CIEPQPF, Department of Chemical Engineering, University of Coimbra

ABSTRACT (Space limited to 2200 characters)

The addition of carbon nanotubes (CNT) to silica aerogels is an interesting route for the mechanical reinforcement of the latter, leading to composite materials not only with greatly improved mechanical resistance but also potentially smaller thermal conductivity, larger surface area and enhanced optical and electronic properties. These materials can be synthesized by the usual sol-gel procedure by mixing a suspension of CNTs (generally oxidized) with a silica precursor solution. However, there are still several mysteries regarding the formation process and the structure of silica-CNT composites. While the formation of a silica aerogel layer around the CNT wall can be observed by electron microscopy, it is unclear if this process is driven by physical forces or by condensation reactions with oxygen-containing moieties, particularly carboxyl, that typically exist at the surface of oxidized CNTs in suspension, and how such interactions affect the structure of the final material. We have provided some answers to these questions by leveraging the ability of molecular modeling and simulation techniques for obtaining physicochemical insights at the atomic and nanoscales. Quantum mechanics calculations, based on density functional theory, have helped shed light on the hitherto unkown mechanism of silanol-carboxyl condensation reactions and compute the associated free energy profiles. On the other hand, classical molecular dynamics simulations, enhanced with the application of the metadynamics algorithm, have allowed the investigation of the physical interactions between primary particles of the silica aerogel and CNTs with different degrees of oxidation, as well as in a solvent mixture of different compositions.

Acknowledgments
This work was funded by Fundação para a Ciência e a Tecnologia (FCT), Portugal, through the granting of a doctoral fellowship (ref: SFRH/BD/136230/2018). This publication is also based upon work from COST Action “Advanced Engineering of aeroGels for Environment and Life Sciences” (AERoGELS, ref. CA18125), supported by COST (European Cooperation in Science and Technology).