



## DLR – DAAD Fellowships

### Fellowship No. 502

**Research Area :** Aeronautics/Space/Transportation/Energy

**Research Topic:** **Computational molecular structure-property investigations of aerogels**

**DLR Institute:** Institute of Materials Research, DLR Cologne

**Position:** Doctoral Fellow

**Openings:** 1

**Job Specification:** This project will take place in the Department of Aerogels and Aerogel Composites at the Institute of Materials Research. Our research group focusses on the synthesis, characterisation (rheology, mechanical testing, thermal properties, electrochemical properties, structural properties (BET, BJH, DFT), chemical sorption, SEM, FIB, TEM, TGA-FTIR, X-ray  $\mu$ CT) and simulations (material modelling, computational mechanics, deep learning) of aerogels and their composites. We are driven by fundamental research as well as an application-oriented one.

This project aims at describing the mechanical and thermal structure-property relationships of aerogels and aerogel composites by means of molecular dynamics simulations. To this end, all-atom and coarse-grained modelling approaches will be used to describe the structural features in different aerogels. A special focus will lie on organic aerogels. Machine learning-based methods will be used to develop predictive models for reverse engineering purposes. The candidate will also work closely with other colleagues working on micromechanical modelling. This is for the effective multiscale description of aerogels and aerogel composites. Innovative approaches within the scope of molecular mechanics are to be developed.

**Required Qualification:** We are looking for a highly motivated PhD student with background in computational molecular mechanics. You have a MSc. degree in chemistry, materials science, mechanical or chemical engineering or similar field. You are experienced in molecular dynamics simulations and

coarse-graining. You have worked with LAMMPS (Large Scale Atomic and Molecular Massively Parallel Simulator). Knowledge of Python is also desired.

**Advantageous Skills:** You are self-motivated, a team player and take personal responsibility.

**English competence:** See requirements on [www.daad.de/dlr](http://www.daad.de/dlr)

Test of English as a Foreign Language (TOEFL): minimum score of 550 (paper version); 90 overall with a minimum score of 22 in Reading & Listening and a minimum score of 21 in Writing & Speaking (Internet version).

International English Language Testing Service (IELTS): minimum overall band score of 6.5 with no component score less than 6.0

**Earliest Start Date:** 01.06.2021

**Application Deadline:** Until position filled

**Further Information:** <http://www.dlr.de>  
<http://www.daad.de/dlr>