The principle aim of this visit is to acquire knowledge on a new type of metal organic framework (MOF) which fabricated by amorphization of the parent crystals. These amorphous MOFS (aMOFS) have been developed in the Membrane Science and Technology Cluster of Twente Universtiy. Preliminary studies suggest that these materials have potential for reversible gas storage and controlled drug release but their potential applications have not been fully explored. This visit will allow to establish a new collaboration by combining experimental and computational methods to fully understand the potential use of these materials for molecular separation.

The detailed atomistic structures of these materials are yet to be identified and within the context of molecular separation, an understanding of the relationship between the material structure and molecular transport becomes vital to predict the performance of these materials for separation of varios mixtures such as CO2/CH4 or CO2/N2. The STMS will focus on the investigation of the structure/separation performance relationship of aMOFs via atomistic level modeling and simulations.

During the STSM, primary focus will be on interpretation the results of structural characterization techniques such as X-ray scattering and thermogravimetric analyses to resolve atomistic structures of the aMOFs. This is the first and crucial step for the modelling of the molecular transport in these materials, since aMOFs do not have a long distance periodic arrangement as in their parent crystal structure, while retaining the primary building blocks. Furthermore, available experimental results on gas separation will be evaluated to set a benchmark for the further modelisation work.

Following the STSM, based on the information acquired during the visit, various atomistic models of various aMOFs materials will be constructed and their framework will be optimized using DFT calculation. Next, guest-host interactions will be investigated for various gas pairs through molecular simulations using Monte Carlo and Molecular Dynamics methods. In conclusion, this STMS will promote a new collaboration between the two parties in the exploration of these new type of materials.