The Membrane Science and Technology Cluster of the University of Twente has been active on different lines of research including “films in fluids”, “soft matter, “fluidics and interfaces”, “inorganic membranes”, “membrane surface science” and “membrane technology and engineering for water treatment”.

During the visit, M.G. Ahunbay delivered a talk to the Cluster members on the typical applications of the materials modeling at the atomistic scale in the field of membrane science. These applications included prediction of structural properties of polymers, crystalline materials and amorphous solids and transport of small molecules in these materials.

The principle outcome of this visit is information acquisition on a new type of metal organic framework (MOF) which fabricated by amorphization of the parent crystals[1]. These amorphous MOFS (aMOFS) have been developed by Prof. Benes’ Films in Fluids group in the Membrane Science and Technology Cluster of Twente Universtiy. Preliminary studies suggested that these materials could be used for thin film fabrication to be used as membrane materials for gas separation. During the visit, available experimental data on aMOF structures were revisited and possible approaches to evaluate structure/property relationship at the atomistic scale were discussed.

Another topic of interest for future collaboration was considered as the transport of ions through perforated graphene membranes[2], which has only a single layer of atoms. These monolayer membranes were developed by the Soft matter, Fluidics and Interfaces group and were reported to show a very similar trend in membrane potential as compared to dense ion-exchange membranes with finite width. The scale of these materials are very suitable for investigations at the atomistic scales.

[1]Cookney, J., Light, M. E., Benes, N. E., & Fila, V. CCDC 1483947: Experimental crystal structure determination. https://doi.org/10.5517/ccdc.csd.cc1lt58v

[2]Ghosh, M.; Jorissen, K. F. A.; Woods, J. A.; Lammertink, R. G. H. (2018). Ion Transport through Perforated Graphene. The Journal of Physical Chemistry Letters, 9, 6339–6344