Postdoctoral Position

"Modelling the interactions between polymers & MOFs"

Position for 1 year - Starting Date: As soon as possible

Keywords: Mixed matrix membranes, Metal-Organic Frameworks, Density Functional Theory, polymers, interfacial interactions

Membranes, due to their low cost, high energy efficiency and ease of processing, have aroused great interest in the field of gas separation. Polymer membranes currently occupy a dominant position in the commercial market, despite the existing tradeoff between permeability and selectivity associated with their use. Over the past decade a novel class of inorganic-organic porous materials, Metal-Organic Frameworks (MOFs), has emerged as a new research domain in solid state materials. These hybrid nanoporous materials formed by the self-assembly of metal ions or clusters, linked together via a variety of bridging ligands, creating stable open structures with sufficiently large pores for industrially-important applications, such as in gas adsorption, storage and separation. Indeed, a number of recent studies have demonstrated that MOFs could be optimal candidates for membrane-based gas separation processes. In addition, owing to the remarkable properties of MOFs, an alternative strategy to overcome the selectivity/permeability trade-off limits of polymer membranes is to make mixed-matrix membranes (MMMs), in which MOF particles are incorporated into polymer matrices.

The success of such an approach would depend on the stability of the mixed matrix membrane created between a given MOF and a polymer. This would in turn depend on the interfacial interaction between the two materials. In order to rationally design such systems, a thorough study of the association of the polymer and the MOF is necessary. This project will deploy a recent software we developed in the group to study the interfacial interactions between MOFs and polymers. In the first instance, the external crystal surface structure of the MOF, and hence the crystal morphology will be determined. Subsequently, the interaction between a given MOF surface and several polymers will then be studied, in order to evaluate the most stable MOF-polymer combinations, to be presented as candidates for fabrication and gas separation testing. Throughout the project, we will maintain a close dialogue with partner expert in the preparation of membranes and the characterization of their performances.

Potential candidates should have a strong expertise in molecular simulations applied to material science.

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