Microstructural Characterization of Charged Polymers Involved in Molecular Mechanisms of Moisture Driven Direct Air Capturing (Mission DAC)

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The Mission DAC project aims to develop affordable and scalable carbon removal by direct air capturing (DAC) to contribute towards the global goal of zero carbon emission. This is a large collaborative project with multiple institutions. Current direct air capturing (DAC) systems mainly depend on energy-requiring heat or pressure changes to overcome the strong attachment of CO_2 to liquid or solid materials that selectively capture CO_2 from the air. Novel anion exchange polymers can capture CO_2 from the air and release it at higher concentrations only with a change in relative humidity; termed a moisture swing. These materials show promise to significantly reduce energy requirements; as the separation is driven by water evaporation. However, they are currently limited by their capacities to capture and transport carbon, and they become mechanically brittle when dry. Our part of the project aims to investigate microstructural characteristics of direct air-capturing polymers through cryogenic focused ion beam (cryo FIB) techniques, and X-Ray scattering techniques. Cryo FIB has not been used previously to characterize these materials and we are currently working on the sample preparation. Our plan is to prepare frozen thin lamella samples at a specified humidity level by cryo-FIB milling to evaluate the structure of the material and the pore sizes. At higher resolution, we will also plan to investigate constraints around the active sites and their distribution when equilibrated over a range of hydration levels in the materials. Thereby, transport pathways responsible for moisture swing may be revealed by visualizing the connectivity of the charged polymer domains using cryo FIB. Structural changes influencing the mechanisms as a function of hydration and CO_2 absorption in moisture swing beads may also be characterized using small-angle and wide- angle X-Ray scattering (SAXS/WAXS) via data collection at synchrotrons and X-Ray free electron lasers (XFELS). Structural investigations will be conducted to probe moisture swing responsive materials to discover suitable, long-lasting, new charged polymers, which can work well in a range of climates and sustain their mechanical integrity. These structural characteristics can provide information for molecular dynamics simulations and the synthesis of new active polymers.

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