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Investigating preferential adsorption of N2 from the air in Zeolite 13X using total neutron scattering

Content

Medical oxygen concentrators (MOCs) utilise pressure swing adsorption to produce oxygen with ~88–92 vol% purity from ambient air. In this process a nitrogen-selective zeolite, most commonly molecular sieve 13X, is first used to adsorb nitrogen from an inlet stream of air at higher pressure (approx. 4 bar), and then subsequent adsorbent regeneration is achieved by passing the air through the sieve at lower pressure (below 1 bar).[1] By operating in fast adsorption-desorption cycles, the machines can produce a continuous stream of oxygen used in oxygen-therapies often prescribed for patients with deprived breathing capabilities.[2]

It has been suggested that the preferential adsorption of nitrogen from the air when compared to oxygen on the 13X molecular sieves is caused by the difference in the quadrupole moment of these two molecules, and the fact that for nitrogen it is three times higher than for oxygen.[3] Consequently, the affinity of nitrogen molecules to the electrostatic field of the zeolite is greater than for oxygen, and results in their enhanced adsorption from the air. Even higher adsorption of nitrogen can be achieved when the Na+ ions present in the zeolite 13X framework are exchanged for Ca2+ or Li+.[1,4]

To gain deeper insights, we conducted total neutron scattering experiments (TNS) to directly probe the molecular arrangement of adsorbates within zeolite 13X under varying pressure conditions. TNS has been proven to be an exceptional experimental tool for gaining insight into the local environment of liquids (e.g. water, benzene)[5,6] and gases (e.g. nitrogen, oxygen, methane) contained within pores of porous media such as MCM-41, and without making crystallographic assumptions.[7,8] Our research contributes to the molecular-level understanding of nitrogen adsorption from synthetic air in zeolite 13X (with Na+ and Ca2+), a critical step in the conscious design of gas-separating solutions.[9] The focus on TNS provides a novel perspective on the behaviour of gases (N2, O2, CO2 and N2/O2 mix) within zeolite 13X pores, offering valuable experimental insights for the enhancement of gas separation processes in healthcare applications.

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