Poster Presentation

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In-situ Gas Dosed Powder Diffraction Under Industrially Relevant Conditions

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The adsorption of small molecules onto functionalized, high surface area microporous materials is important for the advancement of industrial and environmental processes ranging from catalysis and chemical separations, to CO2 sequestration and energy storage. Over the past several years we have focused our research efforts on understanding the molecular interactions of these small molecules with a variety of microporous materials using in-situ powder diffraction methods to correlate structure with chemical properties. Background will be given on the design of gas dosing apparatus for in-situ diffraction studies at synchrotron X-ray and neutron powder beamlines. The result is that accurate doses can be made per quantity of interest (moles of cations, per unit cell, per pore, etc.), or under high pressures (100 bar), and/or chemical reactions can be followed versus temperature/pressure. Several of our recent investigations of CO2/N2/CH4 sorption in cation-exchange zeolites including Zeolite A (5A) and CHA are presented. While many industrial processes use zeolites to carry out these functions, more emphasis has been placed on metal-organic frameworks (MOFs) on late since their properties can be tuned by varying the synthetic components. A number of studies on an isostructural series, M-MOF-74, have been considered investigating why certain functionalization leads to increased specificity for applications such as CO2, O2, CO, and hydrocarbon separations. The ultimate goal is to use the knowledge gained to improve the design of new MOF materials.

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