

## Understanding Selective Propane/Ethane Gas Adsorption using Neutron Diffraction

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Metal organic frameworks (MOFs) offer considerable uses for gas uptake and storage due to their porous nature, chemical tunability, and flexibility. One particular MOF, MUF-16, has recently shown exceptionally high selectivity for carbon dioxide, allowing for potential decreases in energy cost for gas separations. In addition, this MOF also more readily adsorbs propane/propene over ethane/ethylene due to inherent structural flexibility, at STP conditions. We used a combination of in-situ synchrotron X-ray and Neutron diffraction to better understand the structural flexibility and gas interactions. Inelastic neutron scattering, along with calculations, was also conducted to understand the dynamics of the flexibility, highlighting that C<sub>3</sub> molecules more effectively bridge across the framework, inhibiting some types of motion in the material.