

Structural insights into decomposition mechanisms of selected porous materials used for molecular springs

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Molecular springs is a class of functional materials based on porous hydrophobic frameworks immersed and pressurized in a liquid¹. When the system is pressurized over the intrusion threshold, the liquid penetrates into the pores under a constant force, while storing pressure-volume work. A truly remarkable feature of a molecular spring is revealed when the material is depressurized^{1,2}. The intrinsic hydrophobicity extrudes the intruded liquid, recovering the work stored during the compression.

Recent advancement in material science opened up new avenues for investigation of porous systems bringing flexible Metal Organic Frameworks (MOFs) into the hotspot. However, the cornucopia of MOF structures is not paired with their stability under the intrusion-extrusion cycle leaving only zinc imidazolate framework ZIF-8 as the most promising option^{2,3,4}. Unfortunately, ZIF-8 is not completely stable and the mechanism and products of instability are not yet known.

X-ray Absorption Spectroscopy was used to investigate changes of the zinc valence (XANES) and local Zn-coordination (EXAFS) of ZIF-8 from different sources. The results were compared and contrasted to similarly degraded samples of a porous silica gel WC8, this time using Si as the central cation.

The XAS studies were carried out in the transmission mode on the Si-K and Zn-K edges at the ASTRA (former SOLABS) beamline of the Solaris synchrotron.

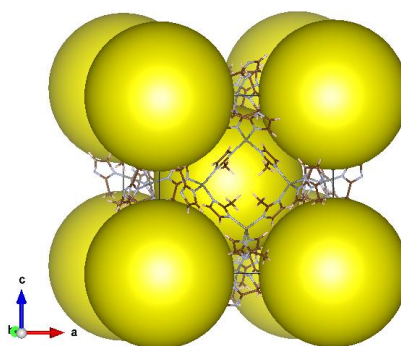


Figure 1. Porous cubic structure of ZIF-8.
Green sphere illustrates size of the cavity.

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