

Pore Architecture of Zeolitic Imidazolate Frameworks: An Investigation Using Positron Annihilation Spectroscopy

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Zeolitic Imidazolate frameworks (ZIFs) are a subclass of metal organic frameworks. ZIFs are shown to have potential application in gas separation, gas storage and sensors. All these applications are based on their nanoporous structure and crystalline frameworks in addition to their high thermal and chemical stability. However, their performance is limited due to their flexible network and gas induced opening of their porous networks. In this regard, it is essential to investigate the modification of their pore architecture under the effect of external stimuli. These studies are proposed to help in design of higher performance ZIFs.

In recent years, we have used Positron Annihilation Spectroscopy to investigate the pore architecture of various ZIFs. These studies are free from any artifacts which may result due to gas-ZIF interactions in case of gas adsorption techniques. The studies have been focussed on investigating the effect of external pressure, crystal size variation and mixed ligands on the pore architecture [1-4]. We have shown that positron annihilation lifetime spectroscopy in combination with slow positron Doppler Broadening Spectroscopy can be successfully used to investigate the pore architecture of these frameworks. These studies have confirmed the existence of a porous network distinct from the amorphous phase of ZIF-8 [1]. It has also been shown that pores in ZIF-8 are interconnected up to ~1.5 micrometre level in case of micrometre size crystals [2]. The crystal size dependence of pore aperture explains the delayed gate opening phenomena in case of ZIF-8 nanocrystals [3]. It has been shown that mixed ligand strategy can be effectively used for tuning of the pore architecture of the frameworks which would result in the improved performance of the frameworks [4].

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[4] P. Utpalla, S.K. Sharma, J. Mor, J. Prakash, J. Bahadur, P.K. Pujari (communicated)