MS038.O01

Metal organic frameworks energy and environmental applications

Praveen Kumar THALLAPALLY[1], James De Yoreo[1], Jun Liu[1], Maria Sushko[1], Debasis Banerjee[1], Jinhui Tao[1], Simon Billinge[1], Sanjit Ghose[1], Maxwell Wesley Terban[1]
[1]*Pacific Northwest National Laboratory, Richland, United States*
E-mail: praveen.thallapally@pnnl.gov

Understanding the mechanism of formation of a new chemical phase, be it a natural or synthetic man-made material from its respective building blocks or reactants is difficult, as often it is not possible to employ traditional in-situ techniques to monitor the formation of the intermediates at their native conditions. To counter the shortcoming of direct visualization, our understanding of material formation pathway largely depends on prediction, which are often retrospective rather than predictive. Complexity of prediction increases with increase in number of reactant components or when thermodynamic parameters such as temperature, pressure are considered. Apart from predictive work by computer simulation, work involving time-dependent ex-situ microscopic and diffraction technique of minerals, pure-inorganic and nanoparticles are commonplace. However, due to the ex-situ nature of the analysis, whether the observation is representative of actual formation pathway is always a cause of debate. For that, in-situ microscopic and diffraction techniques have been developed, while these techniques is sufficient to give an overall idea of the formation pathway of a particular material, they are not essentially good for complex pathways with multiple intermediates in-between. Moreover, many soft materials such as metal organic-framework (MOFs) are prone to electron beam damage, and diffraction techniques cannot infer much information regarding the early stages of nucleation and growth of target particles in terms of shape, size and growth mechanism. This gets particularly challenging when the formation pathway involves amorphous intermediates. MOFs and related materials have many potential applications related to gas-storage and separation, catalysis, bio-imaging and lighting. It is important to understand how they grows in their native conditions to gain further synthetic control over the formation of these materials. My presentation gives an overview of in-situ techniques to understand the formation pathway of a benchmark nanoporous material ZIF-8 in its native formation condition. Further discuss about the gas separation properties of these novel class of materials.

Thallapally et. al., Advanced materials , 2016, Vol.28(18), p.3572-3577
Thallapally, De Yoreo, Liu, Sushko and Jinhui et. al., submitted
Thallapally, De Yoreo, Liu, Sushko, Billinge et. al., submitted

Keywords: MOFs, separation, growth