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Reactive Species Unveiled by Ab Initio Powder Structure Analysis

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Porous coordination network has been the subject of explosive development because of their fascinating properties. However, there is still an unexplored research field in self-assembly of porous materials. There are many metastable states before reaching the thermally most stable state. By controlling the weak intermolecular interactions, we can trap various metastable coordination networks which will not be obtained by conventional thermodynamic control. Kinetically trapped metastable networks were not paid much attention, because firstly it is very difficult to analyze crystal structures. We demonstrated that it is possible to perform ab initio powder structure determination of porous coordination networks using low resolution data; totally different coordination networks can be selectively prepared from the same starting materials by thermodynamic and kinetic control; a robust porous coordination network can be prepared from the kinetic product which can be prepared instantly and in a large scale.[1] We also demonstrated that a pore in porous networks can be used as a crystalline molecular flask.[2] The robust networks maintain crystallinity and enable direct observation of reactive species by X-ray diffraction. It is still challenging to observe reactive species in a pore with clear structural evidence. In this talk, we will report ab initio powder structure analysis of reactive species trapped in a porous coordination network and their unique chemistry.[3]

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