

Microsymposium

MS75.O02

Structural analysis of crystal surfaces of flexible metal-organic frameworks

S. Furukawa¹, S. Kitagawa¹

¹*Kyoto University, Institute for Integrated Cell-Material Sciences (WPI-iCeMS), Kyoto, Japan*

Structural transformability accompanied with molecular accommodation is a distinguished feature of metal-organic frameworks among porous materials. Conventional X-ray crystallography allows for the determination of each structural phase emerged during transformation. However, the propagation mechanism of transformation through an entire crystal still remains in question. Here we elucidate the structural nature of spatial transient state, in which two different but correlated framework structures, an original phase and a deformed phase, simultaneously exist in one crystal. The deformed phase is distinctively generated only at the crystal surface region by introducing large guest molecules, whilst the remaining part of crystal containing small molecules maintains the original phase. By means of grazing incidence diffraction techniques we determine that the framework is sheared with sharing one edge of the original primitive cubic structure, leading to the formation of crystal domains with four mirror image relationships.

Keywords: metal-organic frameworks, Grazing incident X-ray diffraction