

## Microsymposium

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### *Nanoporous Structural Science Developed by the MEM/Rietveld Method*

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Wide-spread functionalization research of Metal Organic Frameworks(MOFs) has brought rapid increase in variety of materials since the beginning of structural study in nanoporous of MOFs were made by SR(Synchrotron Radiation) powder diffraction using the MEM(Maximum Entropy Method)/Rietveld Method(Kitaura et al, 2002). The MEM/Rietveld method has successfully applied to refine the structural position of absorbed molecules and to investigate a bonding nature between the molecules and MOF's pore walls. Noise-resistance electron density mapping with incomplete data set was a key advantage of MEM to visualize unmodeled feature of molecules in nanoporous. Since then, the charge density studies by the MEM/Rietveld Method have uncovered various ordering structure of absorbed molecules into nanoporous more and more(Takata, 2008). Those findings ignited trends to design the nanoporous as the space to be functionalized. Recently, the MEM/Rietveld method has been further developed as the method to map an electrostatic potential and electric field(Tanaka 2006). This technique is making a progress in structural science of MOFs since the visualized electrostatic potential in the nanoporous ought to provide information of interplay between the molecule and the pore walls. The talk will present the recent progress and challenges of the MEM/Rietveld method to the structural science of the MOFs.

[1] Kitaura, R., et al., (2002) *Science*, 298, 2358-2361, [2] Takata, M., (2008) *Acta Cryst. A*64, 232-245., [3] Tanaka, H., Kuroiwa, Y., Takata, M., (2006) *Phys. Rev. B*, 74, 172105.

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