MS03.O02

Application of maximum-entropy electrostatic potential in Materials Science.

E. Nishibori[1]

[1]*RIKEN RSC-Rigaku Collaboration Center, RIKEN SPring-8 Center, Hyogo, Japan*

Charge density (CD) studies by Maximum Entropy Method (MEM) (Sakata & Sato, 1990) from x-ray diffraction data have been widely applied to solve problems and questions in materials science during past two decades. Encapsulations of metal atoms (Takata et al, 1995), gas molecules, as well as protein molecules in the materials have been visualized as MEM CDs. The MEM CD technique is now regarded as a sophisticated technique for visualization in atomic scale. Electrostatic potential (EP) and electric field (EF) from x-ray diffraction data using MEM have been developed in 2006 (Tanaka et al, 2006). The EP & EF successfully applied to ferroelectric material PbTiO3 and a charge ordered manganite system. The method has huge potential in materials science since interaction in the non-atomic region can be visualized experimentally. One of the promising target for EP & EF analysis is host-guest systems, such as porous coordination polymers (PCPs), zeolites, clathrates as well as endohedral metallofullerenes[3]. In the case of host-guest systems, the guest atom(s) or molecule(s) are located in spatially wider sites in comparison to other type of materials. Therefore the detailed structural information in the spatially wider sites is one of the most important issues. In the present study, I present an application of MEM EP & EF analysis to host-guest related system, icosahedral B12 cluster materials and hydrogen adsorbed PCP. The EP studies clearly visualize doping sites in B12 based superconductor and adsorption sites in PCP. The EF enables us to estimate quantitative interaction from host to guest. The quantitative evaluation really bridges between experiment and theory in materials science.

[1] *Sakata, M. & Sato, M. (1990). Acta Cryst. A46, 263-270.,* ***[2]*** *Takata, M., Umeda, B., Nishibori, E., Sakata, M., Saito, Y., Ohno & M. & Shinohara, H. (1995). Nature 377, 46-49.,* ***[3]*** *Tanaka, H., Kuroiwa, Y., Takata, M. (2006). Phys. Rev. B74,172105*

Keywords: Maximum Entropy Method, Electrostatic potential, Charge Density