北京大学量子材料科学中心
International Center for Quantum Materials, PKU

中心系列讲座 ICQM Weekly Seminar Series

Structure determination of zeolites by electron microscopy

Junliang Sun
College of Chemistry and Molecular Engineering
Peking University

Time: 4:00am, Apr. 11, 2012 (Wednesday)
时间：2012年4月11日 （周三）下午4:00
Venue: Room 607, Conference Room A , Science Building 5
地点：理科五号楼607会议室

Abstract

Knowing structures is extremely important for understanding the properties of materials as well as improving their functionalities. X-ray diffraction techniques have been the main method since its invention. Electron microscopy has also played an important role since the development of image processing and simulation. Here we present the recent development of the structure determination by electron microscopy alone and the combination of electron microscopy and powder X-ray diffraction techniques will be also discussed. These methods can be applied for various materials, especially useful for porous materials which are important for catalysis, separation.

One of the most complicated zeolites, IM-5, was first solved by combining powder X-ray diffraction and HRTEM images but its structure can also be directly obtained by 3D reconstruction of HRTEM images.[1] This method can also be applied for solving the structure of mesoporous materials, as we did for IBN-9.[2] IBN-9 shows a unique tri-continuous mesoporous channel system with hexagonal symmetry $P6_3/mcm$. It has the most complex pore structure among all reported mesoporous materials, and is the first representation of H-minimal surfaces in real materials.

For the electron beam sensitive sample, HRTEM images normal show very low resolution, which may not be very helpful for the atomic structure determination, while the electron diffraction requires less stability of the materials. In the structure determination of ITQ-37, the first chiral zeolite with meso pores, electron diffraction intensities were used instead.[3] These intensities were used to pre-partition the overlapped reflections in powder X-ray diffraction to obtain a single-crystal-like diffraction data, which makes the structure solution much easier. For the same reason, one of recent developments of electron microscopy is so-called 3D electron diffraction tomography. This technique can collect the whole diffraction space in an automatic mode, which can then be used for the structure determination as single crystal X-ray diffraction data. For the disorder structure, this technique can also provide useful information in reciprocal space for getting an overview of the materials.[4]

1. J. Sun, X. Zou Review in *Dalton Transaction*, **2010**, *39*, 8355-8362
2. Y. Han, D. Zhang, L.-L. Chng, J. Sun, L. Zhao, X. Zou, J.Y. Ying *Nature Chem.* **2009**, *1*, 123-127.
3. J. Sun, Ch. Bonneau, Á. Cantín, A. Corma, M. J. Díaz-Cabañas, M. Moliner, D. Zhang, M. Li, X. Zou *Nature* **2009**, *458*, 1154-1157.
4. T. Willhammar, J. Sun, W. Wan, P. Oleynikov, D. Zhang, X. Zou, M. Moliner, J. Gonzalez, C. Martínez, F. Rey, A. Corma *Nature Chem.* **2012**, In press

About the speaker

Junliang Sun got his BS and PhD in chemistry at Peking University in 2001 and 2006. After the postdoctoral positions in Cornell University and Stockholm University, he became an assistant professor in Stockholm University in 2009, supported by Swedish Research Council. In 2011, he was selected as one of 1000 young talents in China. Dr. Junliang Sun and his coworkers have published more than 60 publications including four in Nature and its sub-journals. His main research interests are: the synthesis of inorganic porous materials and incommensurate structures; method developments for the structure determination by powder X-ray diffraction and electron microscopy.