Poster

The Development and Application of 3D ED method in Crystalline Porous Materials

Shitao Wu^{1,2}, Yanhang Ma^{1,2}

¹ Shanghai Key Laboratory of High-resolution Electron Microscopy, ShanghaiTech University, Shanghai 201210, P. R. China;
² School of Physical Science and Technology, ShanghaiTech University, Shanghai 201210, P.R. China

wusht@shanghaitech.edu.cn; mayh2@shanghaitech.edu.cn

As a family of functional materials with ordered pores, including zeolites, metal–organic frameworks (MOFs) and covalentorganic frameworks (COFs), crystalline porous materials have presented a wide range of applications in adsorption/separation, electrochemistry and storage, etc [1-3]. The synthesis of novel crystalline porous materials with superior performance requires a comprehensive understanding of their crystal structures at atomic level, thereby establishing reliable structure-property relationships. One of the pressing challenges in this field is the precise structure determination of crystalline porous materials. By applying 3- dimensional electron diffraction (3D ED, Fig. 1a) [4-7], different phases of materials could be identified and classified, and *ab initio* single crystal structure solution could be achieved.

New developments in the 3D ED method, such as automated data collection and high-throughput data processing and analysis, have enabled it to be a more powerful tool in crystalline porous materials structure characterization, which has provided extensive successful examples of crystal structure determination including zeolites/silicates, MOFs and COFs (Fig. 1b) [8, 9].



Figure 1. (a) A schematic diagram of 3D ED (top), with a user interface and a diagram of TEM microscope (bottom). (b) Examples of crystal structures resolved by 3D ED method.

- [1] Jiang, L., Tian, Y., Sun, T., Zhu, Y., Ren, H., Zou, X., Ma, Y., Meihaus, K.R., Long, J.R., & Zhu, G. (2018). J. Am. Chem. Soc. 140 (46), 15724-15730.
- [2] Dong, R., Han, P., Arora, H., Ballabio, M., Karakus, M., Zhang, Z., Shekhar, C., Petkov, P.S., Erbe, A., Mannsfeld, S.C.B., Felser, C., Heine, T., Bonn, M., Feng, X. & Cánovas, E. (2018). *Nature Mater.* 17 (11), 1027-1032.
- [3] Furukawa, H. & Yaghi, O. M. (2009). J. Am. Chem. Soc. 131 (25), 8875-8883.
- [4] Yang, T., Willhammar, T., Xu, H., Zou, X., & Huang, Z. (2022). Nat. Protoc. 17 (10), 2389-2413.
- [5] Kolb, U., Gorelik, T., Kübel, C., Otten, M. T., & Hubert, D. (2007). Ultramicroscopy 107 (6-7), 507-513.
- [6] Ling, Y., Sun, T., Guo, L., Si, X., Jiang, Y., Zhang, Q., Chen, Z., Terasaki, O. & Ma, Y. (2022). Nat. Commun. 13 (1), 6625.
- [7] Wu, S., Li, J., Ling, Y., Sun, T., Fan, Y., Yu, J., Terasaki, O., & Ma, Y. (2022). Chem. Mater. 34 (18), 8119-8126.
- [8] Wang, Y., Peng, R., Sun, W., Li, S., Wu, S., Xu, H., Jiang, J., Chen, S. & Wu, P. (2024). Small, 202307323.

[9] Zhao, Y., Wu, S., Wang, J., Peng, M., Xu, H., Jiang, J., Ma, Y., & Wu, P. (2024). Angew. Chem. Int. Ed., e202318298.

Shitao Wu would thank collaborators from East China Normal University, Zhejiang University, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Science and ShanghaiTech University. Shitao Wu would also thank Chem, School of Physical Science and Technology, ShanghaiTech University for experiments.