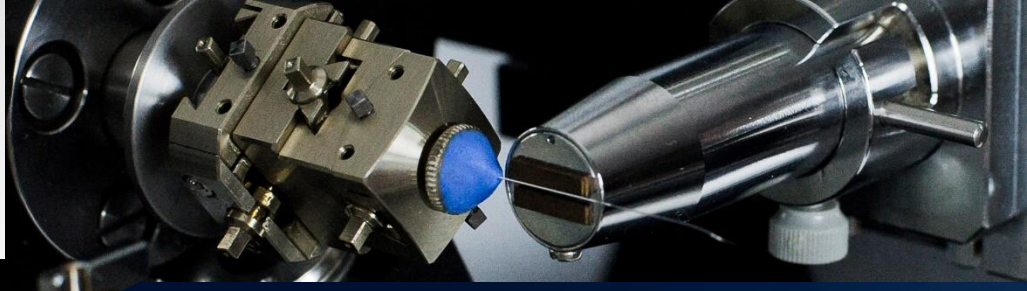
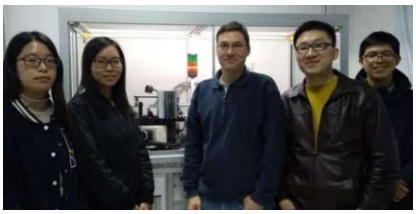


APPLICATION REPORT
STOE STADI P AT DICP OF CHINA



Dr. Peng GUO (second from right) in front of the STOE STADI P in DICP, CAS. Picture taken at the time of installation in 2018.

The research group led by Prof. Zhongmin Liu at Dalian Institute of Chemical Physics (DICP) has focused on the industrial catalysis for more than 30 years, especially for Brønsted acid catalysis. Their investigations are closely associated with industrial catalysts called molecular sieves (MSs), which are a class of crystalline microporous materials with well-defined channels or cavities with pore openings in molecular size.

In order to better understand their crystallographic structure at the atomic level and probe their host-guest interactions, they installed a **STOE STADI P ESSENTIAL** powder diffractometer equipped with a Mythen II detector in 2018.

After the first years of operation, we have asked the structural characterization subgroup, led by Dr. Peng Guo at DICP, to kindly share some of the highlights of the advances made, with us and the STOE community:

Recently, we have accomplished some interesting works regarding MSs, with the assistance of the STOE STADI P instrument:

1. Developing RSS approach for the targeted synthesis of MSs

The targeted synthesis of crystalline microporous silicoaluminophosphate (SAPO) MSs with desired topologies is challenging. Conventionally, the trial-and-error approach assisted by computational methods is widely utilized for this exploration. By analyzing in-house high-quality powder X-Ray diffraction (PXRD) data collected by our STOE STADI P PXRD instrument, we explored an approach called **RSS** (**R**efine, **S**ummarize, and **S**earch) for the targeted synthesis of SAPO MSs. This approach contains three steps:

1) **R**efine known samples against PXRD data and then identify the locations of organic structure-directing agents (OSDAs) and host-guest interactions,

2) **S**ummarize the structural features of OSDA, and

3) **S**earch for suitable OSDA candidates for the targeted synthesize.

By utilizing the **RSS** approach, we have not only extended the synthesis of DNL-6 (**RHO** topology) with nine kinds of OSDAs predicted [1], but also obtained SAPO-42 (**LTA**) using five commercialized amines as OSDA in the fluoride-free system (Figure 1). [2]

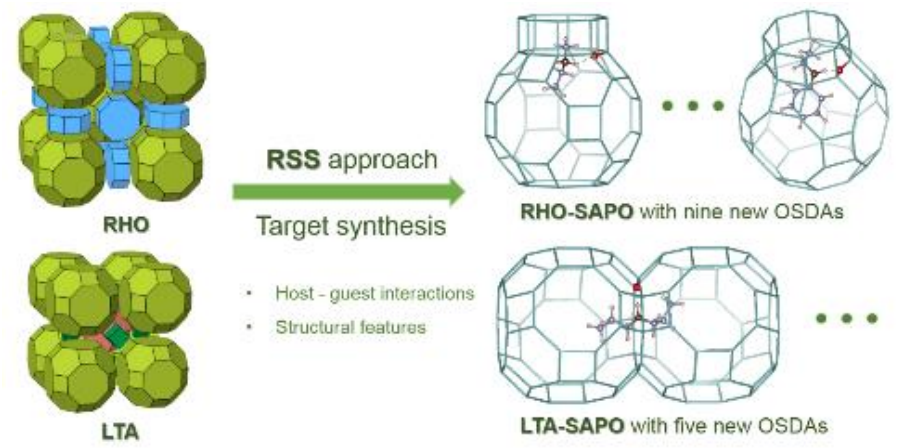
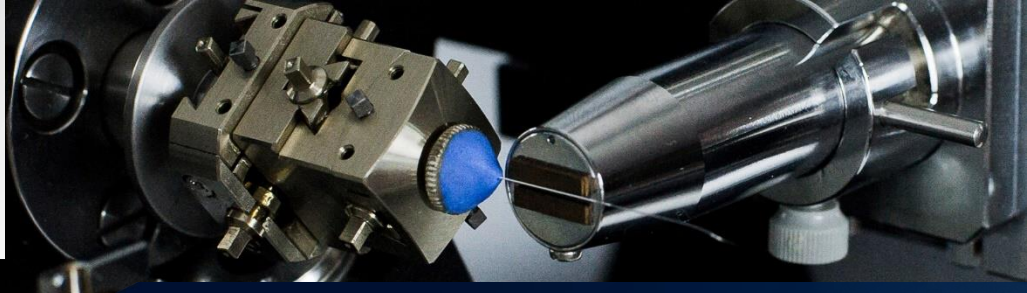


Figure 1. Targeted synthesis of DNL-6 and SAPO-42 by utilizing the RSS method.



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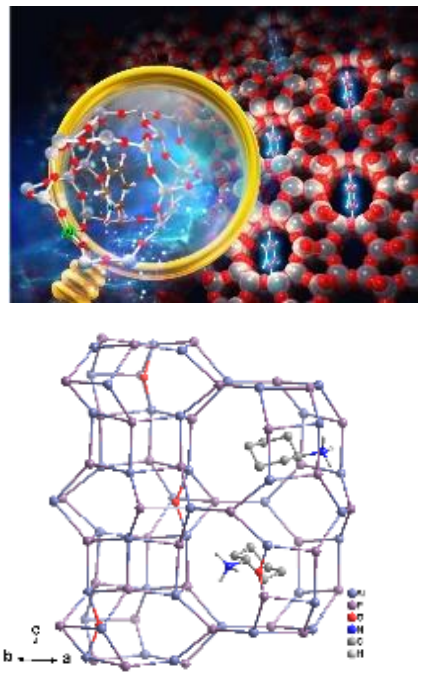

Figure 2. Unraveling the Brønsted acid sites of FER (top) and SAPO-17 (bottom).

2. *Unraveling the Brønsted acid sites*

The crystallographic sites of Brønsted acid in MSs play a significant and unique role in catalysis. Using high-quality PXRD data collected on STOE diffractometer, we unraveled the Brønsted acid sites in aluminosilicate ferrierite (**FER**) zeolite. Through analyzing the refinement results of as-made and pyridine-adsorbed samples, we found that T1 site is an Al-rich position in ferrierite (Si/Al = 26.1) synthesized in a system containing pyridine and Na^+ (Figure 2, left).[3] Moreover, we can also investigate the Brønsted acid sites in SAPO MSs. For instance, we identified the Brønsted acid site (O4) in SAPO-17 (**ERI**) through Rietveld refinement against PXRD data (Figure 2, bottom).[4]

3. *Determining guest inorganic cations*

Except for the proton-type MSs, metal exchanged ones are also applied in many fields. Cu-exchanged MSs have been regarded as the most efficient technology to facilitate selective catalytic reduction of No_x with ammonia (NH_3-SCR). After utilizing Cu-SAPO-42 catalysts for NH_3-SCR, we found that Cu-SAPO-42 catalysts demonstrate the excellent activity even after hydrothermal aging at 800 °C for 16h, which shows much better hydrothermal stability than the commercialized Cu-SAPO-34 catalyst with comparable Si and Cu contents. Then, we identified the active Cu^{2+} ions near the center of single 6-rings of the *lta* cage through Rietveld refinement of Cu-SAPO-42 catalyst (Figure 3).[2]

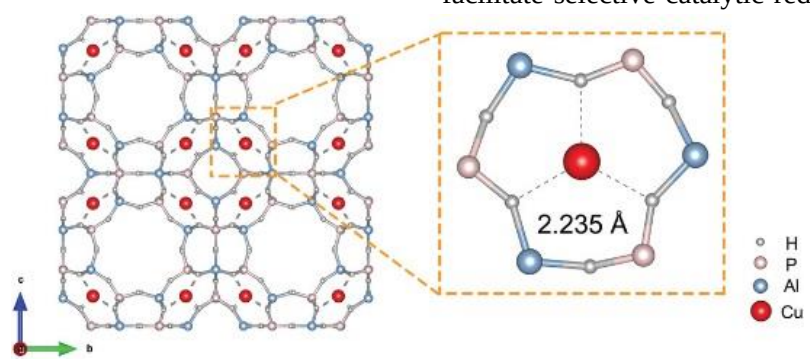

Figure 3. The locations of active Cu^{2+} ions in Cu-SAPO-42 catalyst.

In conclusion, we have gained insightful structural features of our industrial MS catalysts at the atomic level through Rietveld refinement against high-quality PXRD data collected on a STOE STADI P diffractometer. Furthermore, these will facilitate us to build a structure-activity relationship and to identify many more highly-efficient catalysts in the near future. Due to our good user experience, we have introduced STOE powder and single crystal diffractometers in our review.[5]

References

[1] N. Yan, *et al. J. Mater. Chem. A* **2018**, *6*, 24186.
[2] N. Yan, *et al. Small* **2020**, *16*, 2000902.
[3] L. Wang, *et al. CrystEngComm* **2018**, *20*, 699.
[4] X. Liu, *et al. Chinses J. Catal.* **2020**, *41*, 1715.
[5] C. Ma, *et al. Chem. J. Chin. Univ.* **2020**, **accepted**

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Recognizing the referrals of STOE XRDs in their reviews, which demonstrate the contribution of the STOE instrument to their research in this exciting field of science, we are extremely honored to have Dr. Peng and his team in the STOE community.