2019 GSRAC Visit Summary, NSF's ChemMatCARS

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Focus: Structure determination of metal-oxide nanoclusters (polyoxometalates)
Goal: Inorganic materials for a range of industrial applications

My research focuses on a class of metal-oxide nanoclusters known as polyoxometalates (POMs). This class of materials offers rich structural archetypes that are attractive molecular building blocks for making extended structured materials whose properties can be correlated with their structure at the molecular level. POMs have found a range of applications, including sensing, fuel cells, detoxification, medicine, energy storage, and catalysis.

Because of the relatively large number of atoms and complexity of the structures, none of the conventional spectroscopic techniques have been satisfactorily helpful towards resolving these crystals at the atomic/molecular level. The crystals are small and diffraction is weak, leading to poor data sets that cannot be used to resolve the type of crystal structures. With ChemMatCARS's state-of-the-art crystallographic facility at APS (beamline 15-ID-D), high-quality crystal data sets can be collected and structures resolved in minutes by using structural solution and refinement programs and software provided at the facility.

I have been an APS user since March 2017; my research group has been assigned beamtime twice. We were able to resolve some of our structures but not all, as beamtime is a rare opportunity. When Dr. Binhua Lin contacted me to say that my GSRAC application was approved for summer 2019 (6 weeks), I knew it was a dream coming true for me. Not only was I able to collect high-quality data sets on all my samples, I was also able to perfect my experience so that I felt confident collecting data, solving structures for myself, and helping other users from different universities and countries. Other very fascinating experiences were getting to know and appreciate other users' research areas and performing an *in situ* crystallographic study, which has broadened my research focus. Today, I can conveniently build on what I have learnt and boast of a new area of expertise.

My experience would not have been worthwhile without the incredible expertise and personality of Dr. Yu-Sheng Chen (operations manager) and others whom I worked with, including Dr. Siyun Grass Wang (beamline scientist), Dr. Mingjian Zhang (postdoc), Abhishek Ravada (GSRAC fellow), and Natalie Chen (Sector 15 user coordinator).