

## E0012

**Accurate Single Crystal X-ray Charge Density Quality Data Collected at ChemMatCARS, Advanced Photon Source (APS).** Yu-Sheng Chen<sup>1</sup>, T. Graber<sup>1</sup>, P.J. Viccaro<sup>1</sup>, Rasmus Poulsen<sup>2</sup>, Henrik Clausen<sup>2</sup> and Bo Iversen<sup>2</sup>, <sup>1</sup>Center for Advanced Radiation Source (CARS), Univ. of Chicago, 9700 S. Cass Ave. Bldg. 434D, Argonne, IL60439, <sup>2</sup>Dept. of Chemistry & Interdisciplinary Nanoscience Center (iNANO) Univ, of Aarhus, DK-8000 Århus C, Denmark.

Accurate X-ray charge density studies have been collected for single crystal metal-organic framework (MOF, M= Zn and Co) samples with dimensions less than 50  $\mu$ m crystals at low temperature (below 20K) using single crystal X-ray diffraction experiment at ChemMatCARS at the Advanced Photon Source (APS). The high accuracy charge density data were collected using a Bruker 6000 CCD detector, mounted on a HUBER 5020 diffractometer with Pinkerton's type open flow Helium Cyro-system. 30 keV were used for photon energy (wavelength  $\lambda = 0.41325\text{\AA}$ ). The detector settings were  $2\theta = 30^\circ$  and 1 second exposure time using  $0.3^\circ$  phi scans per frame. 2200 and 3200 total frames were collected for each crystal; M=Zn and Co respectively. One data collection was finished within 8 hours. The frames were integrated using SAINT, the oblique correction has been corrected by Oblique software and the data were sorted, averaged, merged and corrected for absorption using the SORTAV program. The  $R_{\text{int}} = 0.0583$  and 0.0562 for M = Zn and Co respectively. The statistical tables from the SORTAV will be presented and the selected deformation and Laplacian maps as well.