

## MS21-P03 | ACCURATE EXPERIMENTAL CHARGE DENSITY DATA: TIPS & TRICKS FOR DATA COLLECTION & PROCESSING

Ott, Holger (Bruker AXS GmbH, Karlsruhe, GER); Ruf, Michael (Bruker AXS Inc., Madison, WI, USA); Kaercher, Joerg; Adam, Martin (Bruker AXS GmbH, Karlsruhe, GER)

A number of recent hardware developments enable scientists working in Quantum Crystallography to collect best ever crystallographic data in shorter time and with utmost convenience. High-brilliance sources, such as the first generation of diamond cooled microfocus sources (I $\mu$ S DIAMOND) and the METAJET providing Indium Ka radiation go along with large active area, mixed-mode photon counting pixel array detectors (PAD) [1] for highest system efficiency.

Despite of all efforts for automation, next to a carefully selected crystal planning and execution of the experiment are of crucial importance. To gain best results from the individual hardware components experimentalists ideally have a certain level of experience and carefully stick to the rules of Good Crystallography Practice (GCP).

This presentation will provide tips & tricks proven to make the charge density research more efficient. These include hints to optimize the instrument performance, but also GCP aspects. The presentation will also highlight recent improvements of the software suites, such as the APEX3 package, with a focus on special options particularly important to the field.[2]

[1] Genoni, L. Bučinský, N. Claiser, J. Contreras-García, B. Dittrich, P. M. Dominiak, E. Espinosa, C. Gatti, P. Giannozzi, J.-M. Gillet, D. Jayatilaka, P. Macchi, A. Ø. Madsen, L. Massa, C. F. Matta, K. M. Merz, P. N. H. Nakashima, H. Ott, U. Ryde, K. Schwarz, M. Sierka, S. Grabowsky, *Chem. Eur. J.* 2018, 24, 10881.

[2] APEX3, Bruker AXS GmbH., 2019.