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National Workshop on Bruker SC-XRD & User Training at Annamalai University, Tamil Nadu, India

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Bruker, in cooperation with Annamalai University, organized the National Workshop on Bruker SC-XRD & User Training for two days from 27-28th September 2019 at the Department of Chemistry, Annamalai University, Tamil Nadu, India. The workshop was mainly focused towards users from the southern part of India (Tamil Nadu, Kerala, and Karnataka). A total of 55 participants from 12 different research institutes/universities attended, some beginners and some experienced.

The objective of the workshop was to bring SC-XRD users together, providing a platform to exhibit/showcase their research work, and provide one-day application training on a Bruker SC-XRD diffractometer, including hands-on training on the latest APEX3 software. The first day of the workshop was dedicated to researchers presenting their work, along with a couple of introductory talks on single crystal X-ray diffraction given by the renowned crystallographers. Hands-on application training on the latest generation Bruker D8 QUEST diffractometer and APEX3 software was offered the second day.

Inauguration of the workshop was carried out in typical Indian tradition by lighting the lamp by **Prof. Guru Row, IISc, Bangalore**, one of the renowned crystallographers in India (expert in X-ray diffraction, Quantum crystallographer and Crystal engineer, also proud user of SMART APEX, KAPPA APEX, SMART APEX II ULTRA for many years) along with **Prof. Kabilan, Dean of Sciences, Annamalai University,** and **Mr. Arin Kumar Chakraborti (Bruker AXS)**. Soon after, **Prof. Guru Row** gave an introductory talk on "Introduction to Single Crystal X-ray Diffraction: Symmetry, diffraction and structure" starting from what are crystals, what is diffraction, Braggs Law, and structure factors, and ending with structure solution. He related Miller indices to a typical "bread loaf" example, and cited a few examples of symmetry in nature. He also explained the technical problems or challenges (such as twinning, disorder, modulated structure, diffuse scattering, etc.) which might be encountered while handling different types of crystals.

Another invited speaker, **Prof. Kumaradhas from Periyar University, Salem** (expert Quantum crystallographer and proud owner of a D8 QUEST ECO and SMART APEX), gave a talk on "Chemical Bonding and Electrostatic properties of molecules from High Resolution X-ray diffraction". He discussed the characterization of chemical bonding

using Quantum Theory of Atoms in Molecules (QTAIM) and gave a few examples of high-resolution data sets, illustrating the electrostatic properties of the molecule. Emeritus **Prof. Meenakshisundaram**, presented the application of "Single crystal XRD analysis in nonlinear optical (NLO) studies", showing how the NLO coefficient depends on the electronic environment, crystal symmetry and exact nature of interacting field components. He also showed that NLO activity depends not only on the molecular structure but also on the crystal packing arrangement. Lastly, he explained the importance of noncentrosymmetric structure for second-order NLO activity.

The afternoon session started with a brief address from the **Registrar** of Annamalai University, followed by **Prof. Thirumaran,** who is in charge of a newly installed D8 QUEST diffractometer at Annamalai University. Prof. Thirumaran presented some latest information on the co crystal structure of zinc-triad dithiocarbamates obtained using the D8 QUEST.

The last session of the day was dedicated to the research students to showcase their research work. Six researchers presented, most on crystal engineering and one on structural phase transitions and superionic conducting property of a Vanthoffite mineral.

The second day of the workshop started with application training by **Dr. Prathapa S. Jagannatha (Bruker AXS)** introducing participants to the newly installed Bruker D8 QUEST diffractometer. He went over the components of the instrument, and explained the difference between various types of X-ray sources (sealed tube & microfocus, Cu, Mo & Ag), and discussed the latest CPAD technology of the Photon II detector, as well as the advantage of larger size detectors. Training participants were briefed on tips and tricks of data collection and processing using APEX3. They collected a couple of data sets in 180 seconds using the fast scan approach and arrived at a final structure using the Auto-structure option of APEX3.

Presenters and other dignitaries (from left to right): Dr. Elancheran, Mr. Arin Chakraborti, Mr. Prakash G. S., Dr. Prathapa S. Jagannatha, Prof. Parameshwaran, Prof. Kabilan, Prof. Guru Row, Prof. Kumaradhas, Prof. Menakshisundaram and Prof. Thirumaran

The second session was hands-on training with the latest APEX3 demo software. Students received two data sets, one regular standard crystal data and one twinned data as provided for training.

Hands-on training using APEX3 included:

- Unit cell determination, data integration, scaling, space group determination and structure solution, structure refinement and **IDEAL** refinement.
- Handling twins with View reciprocal lattice and CELLNOW, multi-domain data integration, scaling using TWINABS to generate two HKL files (HKLF4 and HKLF5) and eventually solving and refining the structure.
- How to handle disordered structure.

The workshop concluded with valedictory function graced by **Prof. Kabilan, Dean of Sciences and Prof. Sankaran, HOD Chemistry, Annamalai University**. **Dr. Prathapa S. Jagannatha** handed out certificates to all the participants and a token of appreciation to the researchers who gave oral presentations. A few participants shared their feedback and experience with the workshop. The next similar kind of workshop or user training from Bruker is planned for the Northern and Western regions of India in the near future.

Bruker wishes to thank **Annamalai University** for hosting the workshop. Annamalai University, accredited with an 'A' Grade by **NAAC** in 2014, is one of India's largest public residential universities, with 10 faculties and 49 departments of study. Sprawling over 950 acres of land, the university does yeoman service in taking education to the doorsteps of the people who are otherwise far from access to centers of higher learning. The university has initiated several innovative teaching programs over the years and has been a pioneer in distance education.

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