AsCA 2024 MALAYSIA

The 18th Conference of the Asian Crystallographic Association

1 – 6 DECEMBER
Kuala Lumpur Convention Centre, Malaysia

Crystallography today:
Beyond the fundamental science

| DAY 1 | | |
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| **CHEMICAL CRYSTALLOGRAPHY** | | **PROTEIN CRYSTALLOGRAPHY** |
| **Single Crystal XRD (Rigaku)** | **Powder XRD (ICDD)** | **Computational Crystallography Data Processing & Model Building (BRUKER)** |

**Single Crystal XRD (Rigaku)**

**MicroED: An Overview**
- Introduction to MicroED (Microcrystal Electron Diffraction)
- Principles and techniques
- Sample preparation for MicroED
- Data collection and processing

**OLEX2: Structural Solving (Professor Horst Puschmann)**
- Introduction and Tips & Tricks with Olex2
- Disorder Modelling using Olex2
- NoSpherA2: Using non-spherical scattering factors
- Identifying problems *before* a structure is submitted for publication

**Powder XRD (ICDD)**

**Part-I: Lecture**
- Powder X-ray Diffraction Method and Applications
- Diffraction Geometry, Systematic Angular errors and calibration procedures, specimen preparation
- Introduction to profile functions, fitting and Quantitative Phase Analysis (QPA) using Rietveld method

**Part-II: Lecture along with hands-on sessions**
- PDF-5+ Database and features overview
- Data mining
- Phase identification methods
- Qualitative and semi-quantitative (RIR) phase analysis
- Advanced phase identification with amorphous components of Trace phases
- JADEPro features overview
- Angular Calibration (Instrument Profile Curve, IPC)
- Pattern Indexing using JADE
- Whole pattern fitting (WPF) and Rietveld refinement

**Computational Crystallography Data Processing & Model Building (BRUKER)**

**Part-I: Lecture**
- Opening & introduction
- Single Cystal X-ray diffraction method & instrumentation overview
- Data Collection: Tips and tricks for efficient data collection
- Data Processing of synchrontron and in-house data

**Part-II: Hands-On**
- Data processing with PROTEUM, including twin recognition and handling
- Summary

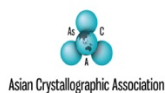| CrysAlisPro: Comprehensive Data Analysis | • Phase identification and Quantitative Phase Analysis (Rietveld) | |
|---|---|---|
| <ul><li>Overview of CrysAlisPro software</li><li>Features and integration with other tools</li><li>Data collection strategies</li><li>Data analysis workflow</li><li>Optimization techniques</li></ul> | • Crystallite Size and Micro-Strain Analysis (time permitting)<br><br>Instructor: Dr. Soorya Kabekkodu | |