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
CHEMICAL CRYSTALLOGRAPHY - **Single Crystal XRD** -
Rigaku

08:00	**Registration**
09:00	**MicroED: An Overview** • Introduction to MicroED (Microcrystal Electron Diffraction) • Principles and techniques • Sample preparation for MicroED • Data collection and processing **Presenters:** Dr Christian Göb Dr Hiroyasu Sato
10:30	**Coffee Break**
11:00	**OLEX2: Structural Solving** • 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 **Presenters:** Dr Horst Puschman

12:30	**Lunch**
13:30	**CrysAlisPro: Comprehensive Data Analysis** • Overview of CrysAlisPro software • Features and integration with other tools • Data collection strategies **Presenters:** Dr Christian Göb Dr Hiroyasu Sato
15:30	**CrysAlisPro: Comprehensive Data Analysis** • Data analysis workflow • Optimization techniques • Q & A Session **Presenters:** Dr Christian Göb Dr Hiroyasu Sato

DAY 1

CHEMICAL CRYSTALLOGRAPHY
- Powder XRD -

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
- Phase identification and Quantitative Phase Analysis (Rietveld)
- Crystallite Size and Micro-Strain Analysis (time permitting)

Presenter:
Dr Soorya Kabekkodu

DAY 1

PROTEIN CRYSTALLOGRAPHY

- Computational Crystallography Data Processing & Model Building -

BRUKER

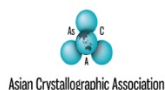|	
08:00	**Registration**
09:00	Opening & Introduction
09:15	Single crystal X-ray diffraction method & instrumentation overview
10:15	**Morning Break**
10:45	Data Collection: Tips and Tricks for Efficient Data Collection
11:45	Data Processing of Synchrotron and In-House Data
13:00	**Lunch Break**
14:00	Hands-On Data Processing with PROTEUM, including Twin Recognition and Handling
16:30	Summary
17:00	End of Day 1

Presenters:
Dr Kenji Yoza
Dr Prathapa S Jagannatha
Dr Zhang Zhenyi