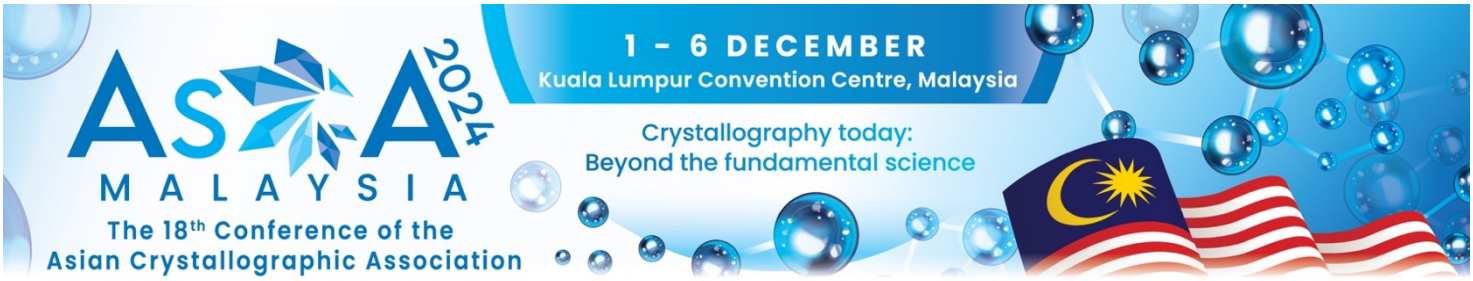

DAY 2

CHEMICAL CRYSTALLOGRAPHY

- Single Crystal XRD -

BRUKER

APEX workshop with hands-on training. The primary topic of this workshop is to teach participants the usage of APEX for data integration, structure determination and refinement from single crystal area detector data. The workshop is open to all applicants interested in the capabilities of APEX.

What you will learn:

- Introduction to the concept and the workflow
- CIRRUS for Sample Submission and Results Dissemination
- Structures within minutes
- Exploring the reciprocal space, defaults, challenges, and pitfalls
- Starting a data collection, tips and tricks
- Indexing including twin handling
- Data integration and scaling
- Structure solutions and refinement including twins, disorder, and others

What you will do:

- Use your own laptop to determine and refine several organic and inorganic structures

Instructors:

Dr Kenji Yoza, Senior Application Scientist SC-XRD, Bruker Japan K.K
Dr Zhang Zhenyi, Senior Scientist SC-XRD, Bruker Shanghai, China
Dr Prathapa S. Jagannatha, Product Manager SC-XRD, Bruker India Scientific Pvt Ltd

DAY 2

CHEMICAL CRYSTALLOGRAPHY
- Powder XRD -

Rigaku

Powder X-ray Diffraction (XRD) is a key technique for analyzing the crystalline structure of materials, helping identify phases, study material properties, and characterize substances like metals, minerals, ceramics, and polymers. The workshop will cover phase identification, crystal structure determination, quantitative analysis of mixtures, and studying properties such as crystallite size and strain.

Additionally, the workshop will address Ab-initio X-ray diffraction, which determines the atomic structure of a material from scratch using only diffraction data and fundamental principles.

With advances in material research, studying amorphous and nanocrystalline materials has become increasingly important. Pair Distribution Function (PDF) analysis in XRD allows for the examination of local atomic structures in both crystalline and amorphous materials, providing insights into their short-range and medium-range order.

08:00 **Registration**

09:00 **Theory of X-ray Diffraction**

- Crystal Lattice, Lattice plane & Plane Indices
- XRD Measurement

Application of XRD

- Phase Analysis
- Crystallite Size
- Crystallinity
- Quantification

10:45 **Coffee Break**

11:15 **Demonstration of**

- Miniflex 600C
- Smartlab Studio II

Sample Testing for participants

12:45 **Lunch Break**

14:15	**Introduction of** • Smartlab XRD • Ab-Initio structure determination via powder XRD • Pair Distribution Function for amorphous & Nano Crystaline Analysis Online demonstration of Smartlab XRD
16:30	**Coffee Break and Discussion** **Instructors:** Dr Muhammad Firdaus Bin Omar Dr Low Yiin Jian Mr Takahiro Kuzumaki Mr Yuji Shiramata

DAY 2

PROTEIN CRYSTALLOGRAPHY

- Computational Crystallography Data Processing & Model Building -

08:00	**Registration**
09:00	X-ray Diffraction Experimentation
10:30	Introduction to CCP4 Cloud
11:00	**Coffee Break**
11:15	CCP4 Cloud • Data processing with Xia2 • Molecular replacement basics Model preparation for molecular replacement (AlphaFold, Assemblies, Pruning and other modifications)
13:15	**Lunch Break**
14:00	**Hands-On** • Solving a structure with MR (Software, what to look at for confidence of the solution, or for signs of failure) Refinement and model completion
16:30	Summary & Closing
17:00	End of Day 2

	Presenters: Dr Ruslan Sanishvili Eugene Krissinel Andrey Lebedev Ronan Keegan

Organised by: MALAYSIAN CRYSTALLOGRAPHIC ASSOCIATION

Co-organised by: Asian Crystallographic Association

Supported by: Malaysia Convention & Exhibition Bureau; Meet in Malaysia BE Greater, Together.; Malaysia Truly Asia

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