

## REGISTRATION FEES

**Early bird** (before 31 January 2020): **RM750.00**

**Normal** (until 14 February 2020): **RM800.00**

Registration will get a **FREE** SCXRD Analysis for one sample

## MODE OF PAYMENT

**Bank draft/cheque** must be made to:  
Bendahari Universiti Putra Malaysia

*Payment Reference:* <name> **CRYSTALS**

### Electronic Funds Transfer (EFT)

Beneficiary Name: Bendahari Universiti Putra Malaysia

Bank Name: CIMB BANK BERHAD

Account No. : 8002151963

SWIFT Code: CIBBMYKL

Payment Reference: <name> **CRYSTALS**

### VOT (For UPM Staff and Students ONLY)

VOT number for payment **62069**

**Registration** can be made at:  
<https://forms.gle/Fh5kQ1YTtogZ5jTi9>

Please email the proof of payment to:  
**ibra@upm.edu.my**

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## CRYSTALS WORKSHOP FOR BEGINNERS: FROM DIFFRACTION DATA TO COMPLETE STRUCTURE SOLUTION

**17<sup>th</sup>-19<sup>th</sup> FEBRUARY 2020**

**BILIK SAINTIS GEMILANG,  
FACULTY OF SCIENCE,  
UNIVERSITI PUTRA MALAYSIA.**



## INTRODUCTION

Single-crystal X-ray Diffraction (SCXRD) is a non-destructive analytical technique which provides detailed information about the internal lattice of crystalline substances, including unit cell dimensions, bond-lengths, bond-angles, and details of site-ordering. Directly related is single-crystal refinement, where the data generated from the X-ray analysis is interpreted and refined to obtain the crystal structure.

**CRYSTALS** is a software package for single crystal X-ray structure refinement and analysis which is FREELY distributed over the internet. **CRYSTALS** aims to provide novice users with the expert decision-making tools required for undertaking unsupervised structure determination. The **CRYSTALS** software can be downloaded from <http://www.xtl.ox.ac.uk/crystals.1.html>.

## OBJECTIVES

- ◆ To give participants an understanding of the basic theory and application of SCXRD.
- ◆ To demonstrate the use of **CRYSTALS** software in molecular structure analysis from X-ray diffraction data to absolute molecular structure.
- ◆ To be able to diagnose and solve problems in SCXRD solution of difficult structures

## WHO SHOULD ATTEND?

Researchers and graduate students who are involved in synthesising new compounds which need determination of molecular structure through single-crystal X-ray diffraction technique.

## OPPORTUNITIES

- Meet and greet with the experts in this field
- Update on new techniques of SCXRD
- Networking opportunities with researchers and experts within Malaysia and regionally

## TENTATIVE WORKSHOP SCHEDULE

Date	Topics
Monday, 17 <sup>th</sup> February 2020	X-ray diffraction, data collection, symmetry Structure solution and refinement Introduction to <b>CRYSTALS</b>
Tuesday, 18 <sup>th</sup> February 2020	Assessment of results: Fourier maps Advanced refinement: disorder Refinement of disordered materials Production and pre results
Wednesday, 19 <sup>th</sup> February 2020	Advanced refinement: absolute structure Twinning, diagnosing problems Absolute structure examples Twin examples and other problems

## SPEAKER



### Assoc. Prof. Dr. Richard Cooper

Head of the Chemical Crystallography Unit,  
University of Oxford, UK

Co-writer for the **CRYSTALS** software package for single-crystal X-ray structure refinement and analysis

<http://research.chem.ox.ac.uk/richard-cooper.aspx>

Dr Cooper followed a Chemistry MA from Oxford with a DPhil in Crystallographic Computing in the research group of Dr David Watkin. After research posts in academia and industry he returned to the Department of Chemistry, University of Oxford in 2010 as Head of Chemical Crystallography and Associate Professor. His research interests include crystallographic structure analysis and application of machine learning classification methods to crystallographic data. Dr Cooper is responsible for the development and distribution of the crystallographic analysis software **CRYSTALS**. He also is currently a co-editor of Acta Crystallographica Section C.

