

# IYCr 2014 Open Lab Hong Kong



**3-7 December 2014**

## Background

The year 2014 has been marked out by UN as “The International Year of Crystallography”. The arrangements for this were first publicized at the Asian Crystallographic Association meeting in Hong Kong which was held on 7-10 December 2013. Now that the year is drawing to a conclusion, it is perhaps fitting that one of the final official functions of the IYCr2014 will be an OpenLab to be held in the beautiful HKUST campus in Clear Water Bay. The OpenLab HK will be a 5-day workshop / school in chemical crystallography and is primarily intended for young scientists from around the region who are researching in the field. Participation numbers are strictly limited, since the workshop will have a number of practical as well as theoretical and discussion sessions. It is anticipated that non-local participants will be limited to 20-25 and local participants around 10-15 persons. To apply for a place, please fill out the registration form, and send asap by E-mail to [chwill@ust.hk](mailto:chwill@ust.hk) or FAX to +852-2358-1594. Registrants will be notified by E-mail on the status of their application.



The entrance piazza of Hong Kong University of Science and Technology



### **OpenLab HK Fees**

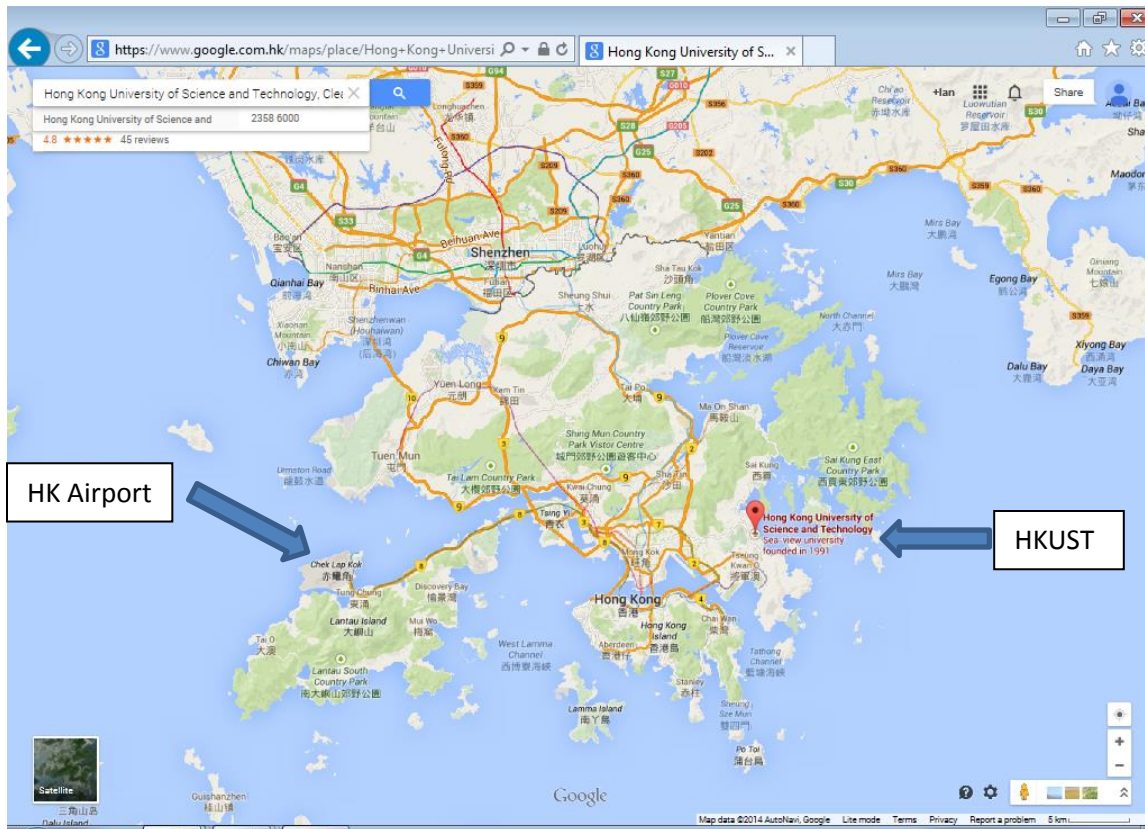
Due to the generous support of sponsors such as the International Union of Crystallography (IUCr), UNESCO, Agilent Technologies and HKUST, and in keeping with other IYCr2014 OpenLabs around the world, no fees will be charged to attend the OpenLab HK. However a charge of US\$300 is necessary as a Residential Fee for a single room (part of 3-bedroom apartment) on the HKUST campus for 6 nights (2 to 7 December). Breakfast, lunch and morning / afternoon snacks and a workshop dinner will be included for participants. Since space is limited, residential fees must be received in order to confirm your workshop place by the deadline of 15 November 2014.

### **General Information**

The weather in Hong Kong in early December is usually pleasant; moderately warm and dry. Participants should check the detailed forecast before attending, since a range of conditions are possible. Hong Kong is well-known as a regional hub for air travel and should be readily accessible from most major cities of Asia. The workshop is being held in early December and should not be subject to high season fares, which can rise steeply near to the Christmas and New Year holiday break. It is anticipated that most non-local participants will enter Hong Kong via the international airport.

### **Transportation to HKUST**

In Hong Kong taxis are quite a reasonable price and from airport will cost around HK\$300 (US\$40) which is not bad for a 30 km 1 hr journey. Hong Kong also has an excellent public transport system. For details of getting to HKUST see [http://ihome.ust.hk/~meyklee/HKUST\\_direction.jpg](http://ihome.ust.hk/~meyklee/HKUST_direction.jpg)



LOCATION MAP  
THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY



MTR Stations with bus or green minibus service to HKUST  
提供往科大巴士或綠色專線小巴服務的港鐵車站

Diamond Hill 鑽石山:	91, 91M
Choi Hung 彩虹:	91, 91M, 11, 11S
Ngau Tau Kok 牛頭角:	104
Tiu Keng Leng 調景嶺:	792M
Hang Hau 坑口:	11, 11M, 11S
Po Lam 寶琳:	91M

Transportation from airport to HKUST:  
For passengers with bulky luggage, taking a taxi to HKUST direct is recommended.  
Those with simple luggage may take Airport Bus A22 to Lam Tin, and change for taxi to HKUST.

Bus Routes 巴士路線  
Green Minibus Routes 綠色專線小巴路線

## HKUST Campus

The university campus is relatively straightforward to get around once you are familiar with it. Accommodations will be in the University Center, which is separate from the main academic building which is marked with the red circle in the map below.



Further details for accommodation and registration arrangements will be sent later.

Participants should arrive to Hong Kong on Tuesday 2 December and check in in the afternoon at the North Block of the University Center, HKUST. The reception desk is open from 08.00-22.30. There will be a Welcome Mixer on evening of 2 December.

The workshop itself will begin in the morning of 3 December and will run through to Sunday afternoon 7 December. Participants must check out of their rooms by Monday 8 December 12.00 noon.

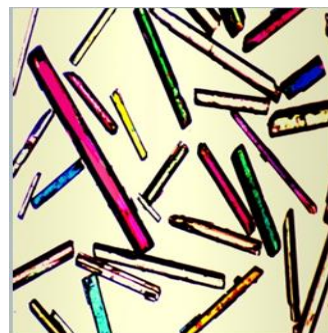
## Program and Itinerary

A detailed timetable will be sent in November, however the topics to be covered will include:

- 1. Crystal Growth – Theory and Practice**
- 2. Basics of X-ray Diffraction, Crystals and Symmetry**
- 3. Structure Determination Overview**
- 4. Selecting and Mounting Crystals**
- 5. Diffractometer I. Pre-experiment:  
Unit cell and Space group determination**
- 6. Diffractometer II. Data Collection and Reduction**
- 7. Using the OLEX2 Software Package**
- 8. Structure Solution and Refinement**
- 9. Validation, Tables and Figures**
- 10. Databases and Publication**
- 11. Special Topics**

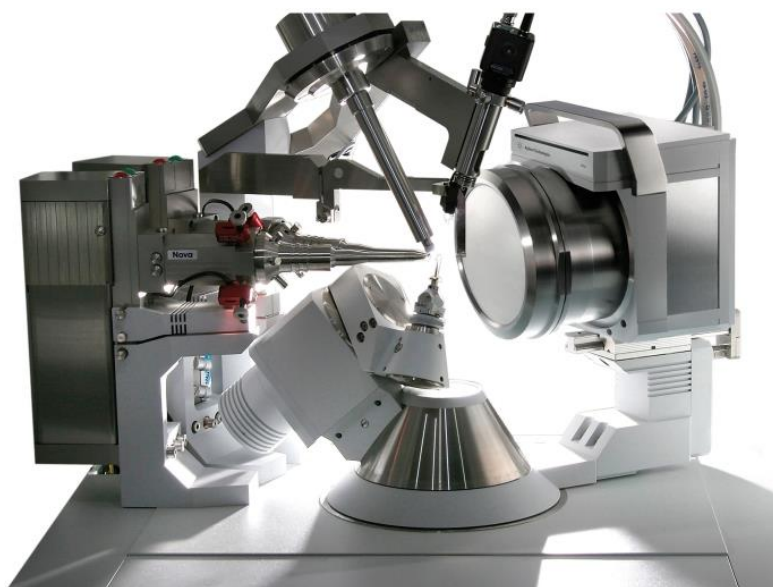
## Working with Your Own Samples

Practical tutorials on growing, selecting and mounting crystals will be conducted at the beginning of the course. Those participants wishing to collect diffraction data on their own sample are encouraged to do so. They should please contact the organizers ahead of time to arrange this and send sample specimens, or materials for crystallization (maximum of two sample types) at least 2 weeks ahead of the workshop. Ideally samples should be non-solvated, non-volatile and non-hazardous. Where possible relevant MSDS sheets should be included for any samples sent.



## Agilent Diffractometers

Two dual wavelength single crystal diffractometers – Agilent Gemini and Agilent Supernova instruments will be available in the workshop for practical demonstration classes and collection of diffraction data. Dr. Fraser White of Agilent Technologies will lead lab demonstrations in the use of the instruments, assisted by Dr. Herman Sung, who is in charge of the X-ray diffraction laboratory at HKUST.



Agilent Youtube video: <https://www.youtube.com/watch?v=ELWtEU-br60>

The OpenLab HK is intended in part for complete novices who have no prior experience of using such equipment, so don't worry if it all looks complicated! The choice of Molybdenum versus Copper X-radiation will be discussed, as well as the optimal conditions for collecting diffraction data on various samples. These will include organic, inorganic and hybrid solids and also chiral samples requiring absolute structure determination.

## Olex2 Software

The OpenLab HK will incorporate a workshop on the use of the powerful crystal structure software package Olex2. This will be presented by Dr. Horst Puschmann of OlexSys. Little or no previous knowledge of the software is assumed, though many tips and advanced techniques will be provided for existing users.



Olex2 is a powerful tool for small molecule crystallography designed to be simple to use for novices users whilst providing complex functionality and tools for experts.

### Solution & Refinement

- Choice of solution & refinement programs, full ShelX support
- GUI or command-line input
- History: Return quickly to previous solutions / refinement

### Advanced Tools

- Easy restraints & constraints
- Advanced disorder modelling tools
- Interactive electron density maps
- Integrated solvent masking
- Data analysis plots

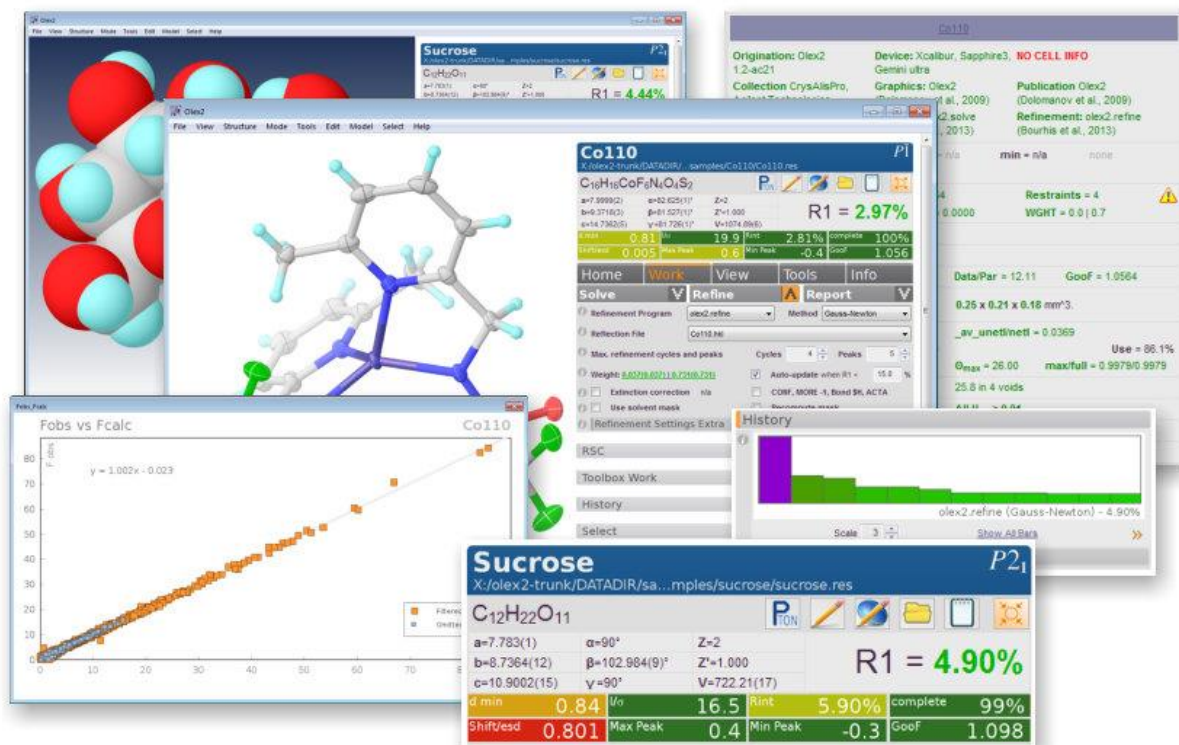
### Structure Images

- Multiple atom display styles
- Easy and accurate labelling
- Symmetry generation & packing
- Publication-quality output

### Report & CIF Generation

- One click report generation
- Customisable reports
- Easy table production for papers
- Automatic CIF synchronisation

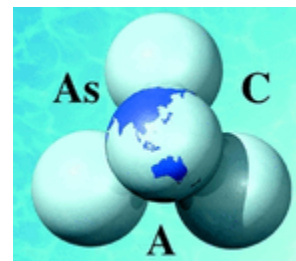
[www.olex2.org](http://www.olex2.org)



Participants are requested to download a version of Olex2 on their laptop computer before attending the workshop. It is available for free for both Windows and Mac platforms from the website [www.olex2.org](http://www.olex2.org).

### IUCr Regional Affiliation: AsCA

The International Union of Crystallography aims to promote the science of crystallography around the world. Its regional affiliate is the Asian Crystallographic Association (AsCA). The OpenLab HK offers an opportunity to provide impetus to develop the science and its practice in some of the less developed countries of the Asian region. With the relatively low costs we encourage participation from countries with relatively less research support. In exceptional cases, some limited travel bursaries may be available and request for this should be made of the organizers when submitting the Registration form. Applications to attend from outside the AsCA region are also welcomed, but in such cases note that travel support cannot be provided.





## Organization

### IYCr2014 OpenLab HK

*Chairman:* Prof. Ian WILLIAMS,  
Department of Chemistry,  
HKUST, Clear Water Bay,  
Kowloon, Hong Kong  
E-mail: [chwill@ust.hk](mailto:chwill@ust.hk)



Prof. Ian WILLIAMS



Prof. Michele ZEMA

*IUCr Representative:*  
Prof. Michele ZEMA  
International Union of Crystallography  
5 Abbey Square  
Chester CH1 2HU, England  
E-mail: [mz@iucr.org](mailto:mz@iucr.org)

## Lecturers

Dr. Fraser WHITE	Agilent Technologies, Oxford, U.K.
Dr. Horst PUSCHMANN	OlexSys, Durham, U.K.
Dr. Alison EDWARDS	ANSTO, Australia
Prof. Michele ZEMA	IUCr, UK and U. Pavia, Italy
Prof. Ian WILLIAMS	HKUST, Hong Kong

## Demonstrators

Dr. Herman SUNG	HKUST, Hong Kong
Dr. Lawrence WONG	HKUST, Hong Kong
Dr. Yan ZHOU	HKUST, Hong Kong



*View of HKUST Campus from the sea... hope to see you here in December!*