

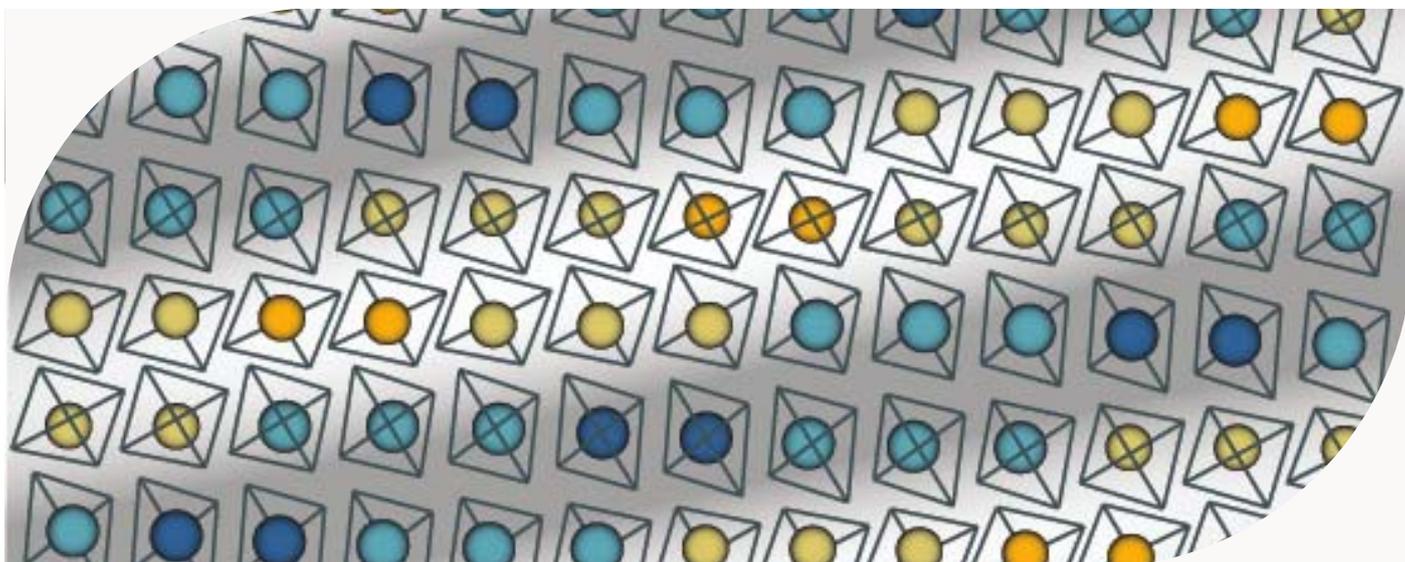


Aperiodic Crystals for Beginners

IUCr Satellite meeting

Wednesday 31 August - Thursday 1 September 2011

Alcalà de Henares, Spain



Presentation

Aperiodic crystals (incommensurately modulated phases, incommensurate composite crystals and quasicrystals) are found in many different systems such as minerals, the elements at high pressures, various inorganic compounds, molecular crystals and intermetallics. Their identification is nowadays easier thanks to the steady improvement of instrumentation, modern X-ray and neutron detectors and advanced transmission electron microscopes. The knowledge of the atomic structure of aperiodic crystals is a key point for the understanding of their chemical and physical properties. However, this still remains difficult for the non-specialist. This two-day satellite meeting offers a basic and tutorial introduction to structural analysis of aperiodic crystals. The general concepts of the high-dimensional crystallography will be introduced step by step and they will be applied to a few organic and inorganic materials

Location

The satellite meeting will take place in Alcalà de Henares, a beautiful historical Spanish city, conveniently located about 30 minutes from the Madrid international airport.

Organizing committee

M. de Boissieu (Chair), M. Perez Mato (co-chair), A. Abakumov, G. Chapuis, M. Dusek, M. E. González Mosquera, S. van Smaalen.

Scientific Advisory Board

The IUCr commission on Aperiodic crystals

Lecturers

A. Abakumov, University of Antwerp, Belgium
G. Chapuis, EPFL, Lausanne, Switzerland,
M. de Boissieu, SIMaP, CNRS, Grenoble, France
J. Haderman, University of Antwerp, Belgium
S. van Smaalen, Bayreuth University, Bayreuth, Germany
H. Takakura, Hokkaido University, Japan

Lecture content

- 1- *Introduction to aperiodic crystals* (1:30)
 - How to recognize aperiodic structure
 - Diffraction pattern and indexing
 - Various type of aperiodic order
 - Examples of different materials
 - Example of the sinusoidally modulated chain explained in details.
- 2- *Introduction to superspace crystallography* (1:30)
 - A simple 1D - 2D example such as the sinusoidally modulated chain.
 - Concept of superspace group
 - Modulation functions and their symmetry properties
 - Structural parameters and t plots
- 3- *Tutorial: Example of displacive incommensurate modulations:* (2:00)

A simple example treated step by step in *tutorial*:

 - Diffraction pattern, indexing and symmetry determination
 - Determination of the basic structure and modulation parameters
 - Refinement
 - Interpretation

Organic or inorganic compound
- 4- *Introduction to quasicrystals* (2:00)
 - Discovery of QC. Definition of QC
 - Family of QC/ samples.
 - Fibonacci chain and 1D-2D example / differences with incommensurate
 - Characteristic of diffraction pattern
 - Basis of structure determination.
- 5- *Example of composite structure* (1:30)
 - Composites structure
 - Direct and reciprocal space: comparison with incommensurate structures
 - Symmetry aspects
 - Modeling
 - Refinement and interpretation
- 6- *Icosahedral quasicrystals* (1:30)
 - Icosahedral quasicrystal
 - Example of the CdYb QC
 - Step by step structure determination.
- 7- *Tutorial: Example of incommensurate modulations* (2:00)

A simple example of step-like occupational modulation

 - Diffraction pattern
 - Modeling the structure with the crenel functions
 - Combination of occupational and displacive modulations
 - Refinement
 - Interpretation

Accommodations



PARTNER CISNEROS HOTEL

Located only at 5 minutes walk distance from the historical centre of the town. The Hotel has 42 rooms with complete bathrooms, air conditioning, satellite TV and channel bonus, hairdryer, restaurant and parking

Prices per room (including lodging, breakfast and VAT (8%)):

- Single room: 50.47 €
- Double room: 50.47 €.

Address:

Paseo de Pastrana, 32
28803 Alcalá de Henares
Tel.: +34 91 888 25 11
Fax: +34 91 883 19 95



SAN ILDEFONSO RESIDENCE (University Residences)

This Residence is located in the Central courtyard of the Cisneriana building of the Rectorate of the Alcalá University (Old Cisneriana University).

Two-floored building with 41 rooms with fully equipped bathroom, heating, satellite TV and fax service.

The Residence does not have breakfast service but in the first floor has a living room equipped with television and a free service of coffee, tea and biscuit.

Prices per room (including accommodation and VAT (8%)):

- Single room: 45.42 €.
- Double room: 45.42 €.

Address:

Plaza San Diego,
28801 Alcalá de Henares. Madrid
Tel: +34 91 878 81 46
Fax: +34 91 889 37 16



Registration and deadlines

Registration fees.

Student or young scientists (under 30 years old):	130.00 €
Academic researchers:	230.00 €
Full registration:	500.00 €

The registration fee covers the welcome party, two lunches, the satellite meeting dinner and coffee breaks. The registration fee has to be paid using the registration form. Hotel reservation is to be carried out separately using the form. Prices are about 50 €/night, the room can be shared.

Deadlines.

Registration and hotel booking: July 10th 2011

Contacts

e-mail : crystals2011@fgua.es; Marc.de-Boissieu@simap.grenoble-inp.fr
website: <http://sig3.ecanews.org/aperbeg2011/aperbeg2011.htm>.

Tel : 33 (0)4 76 82 65 18
Fax : 33 (0)4 76 82 66 44

