

International Workshop on Fundamentals of Crystallography

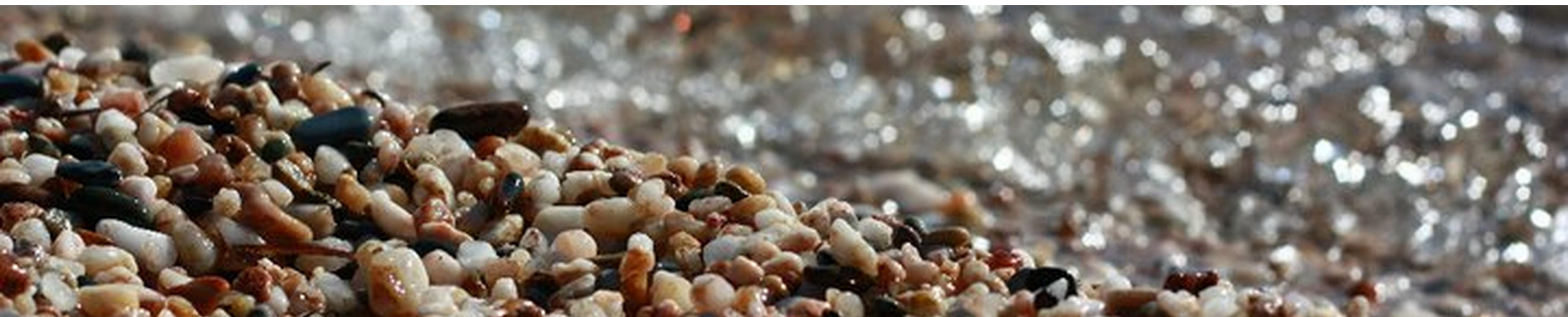
University of Patras (UPAT), Greece April 1-7, 2013

Achaia Beach Hotel - http://www.airotel.gr/greek/hotel/achaia_beach_hotel

http://epdic.ing.unitn.it/2013_Workshops_at_the_University_of_Patras.pdf

The determination of the 3D structure of materials at the atomic scale is crucial for understanding their physical, chemical and biological properties. Such information is obtained from crystallographic studies, that have advanced enormously since their advent using X-ray diffraction 100 years ago. The construction of powerful neutron and X-ray sources (synchrotron and free electron laser facilities), with refinement of experimental methods for structural studies, improvements in detectors, and the huge increase in computational capabilities, have contributed to marked progress in recent years. This school will provide an extensive training in both theoretical and practical aspects of modern crystallography.

The school will be followed by the International workshop on X-ray Powder and Electron Crystallography (8-12 July 2013, University of Patras, Greece).



Tutor

Carmelo Giacovazzo, Institute of Crystallography, Bari, Italy

Organising Committee

Irene Margiolaki, UPAT, Patras, Greece

Georgios Spyroulias, UPAT, Patras, Greece

Irene Mavridis, N.C.S.R. "DEMOKRITOS", Athens, Greece

Carmelo Giacovazzo, Institute of Crystallography, Bari, Italy

Stavros Nicolopoulos, NanoMEGAS, Brussels, Belgium

Fabia Gozzo, Excelsus Structural Solutions S.P.R.L, Brussels. Belgium

Local Organizing Committee , UPAT:

Athanasios Galanis

Partha Pratim Das

Mary Kollia

Fotini Karavassili

Anastasia Giannopoulou

Elena Kotsiliti

Alexandros Valmas

Kon/na Magiouf

Stavroula Fili

Limited Number of Participants. Registration Fee 100 Euros, Registration Deadline: 30th January 2013

Student Bursaries Available. . For registration and/ or bursary application email: partha@upatras.gr

Applications should include CV, letter of interest and one reference letter



International Workshop on Fundamentals of Crystallography

University of Patras (UPAT), Greece April 1-7, 2013

Conference and Cultural Centre

PROGRAM

Mandatory: the careful study of the first 12 pages of “Fundamentals of Crystallography” plus exercises assigned by Carmelo Giacovazzo prior to the lectures! Material distributed by organizers. The accepted participants are invited to contact Carmelo by email, at the address carmelo.giacovazzo@ic.cnr.it for discussing and overcoming difficulties during the homework.

Time	April 1 Monday	April 2 Tuesday	April 3 Wednesday	April 4 Thursday	April 5 Friday	April 6 Saturday	April 7 Sunday
8:30-10:00	Opening & Discussion of the student home-works	The Bravais lattices	The mathematical model of lattice	X-ray, neutron and electron scattering	Scattering from a molecule	Symmetry in reciprocal space <u>Part II</u>	The Fourier synthesis and the phase problem
10:00-10:30	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
10:30-12:00	Lattice periodicity and symmetry restrictions	The space groups <u>Part I</u>	The concept of convolution	Thomson scattering	Diffraction by crystals <u>Part I</u>	Systematic absences	Difference and hybrid Fourier syntheses
12:00-12:30	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break	Closure
12:30-13:30	Point groups <u>Part I</u>	The space groups <u>Part II</u>	The concept of Fourier Transform <u>Part I</u>	Interference of scattered waves	Diffraction by crystals <u>Part II</u>	Space group determination	
13:30-15:00	Lunch	Lunch	Lunch	Lunch	Lunch	Lunch	
15:00-16:00	Point groups <u>Part II</u>	The space groups <u>Part III</u>	The concept of Fourier Transform <u>Part II</u>	Scattering by atomic electrons and by atoms	Bragg's law, reflection and limiting sphere	Diffraction by real crystals	
16:00-16:30	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break	
16:30-17:30	Laue classes	The space groups <u>Part IV</u>	Fourier transforms and convolutions	The temperature factor	Symmetry in reciprocal space <u>Part I</u>	Diffraction intensities and structure factors	
18:00-22:00	Welcome Ceremony					Music Evening*	

***Concert at the Conference and Cultural Centre- UPAT:** Musical performance with the outstanding Argentinian solist Mario Stefano Pietrodarchi and the Orchestra of Florence.
Organization: Patras Tango Academia. April 6, 2013.

International Workshop on Powder & Electron Crystallography

University of Patras (UPAT), Greece July 8-12, 2013

Conference and Cultural Centre

http://epdic.ing.unitn.it/2013_Workshops_at_the_University_of_Patras.pdf

Tutors

Detlef Beckers, PaNalytical, Almelo, The Netherlands

Corrado Cuocci, Institute of Crystallography, Bari, Italy

Andrew N. Fitch, ESRF, Grenoble, France

Mauro Gemmi, IIT@NEST, Pisa, Italy

Carmelo Giacovazzo, Institute of Crystallography, Bari, Italy

Fabia Gozzo, Excelsus Structural Solutions S.P.R.L, Brussels. Belgium

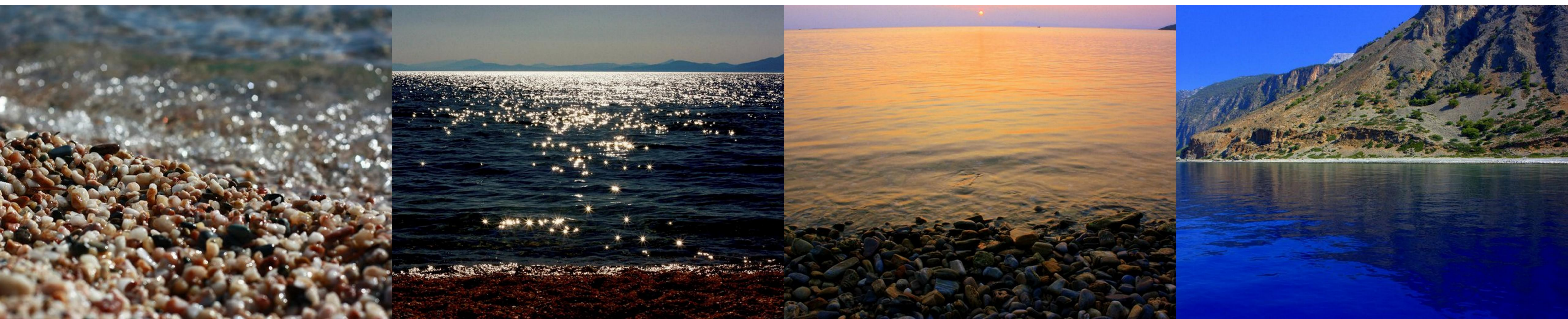
Irene Margiolaki, UPAT, Patras, Greece

Stavros Nicolopoulos, NanoMEGAS, Brussels, Belgium

Rosanna Rizzi, Institute of Crystallography, Bari, Italy

Robert B. Von Dreele, APS, Argonne National Laboratory, Chicago, USA

Jonathan P. Wright, ESRF, Grenoble, France



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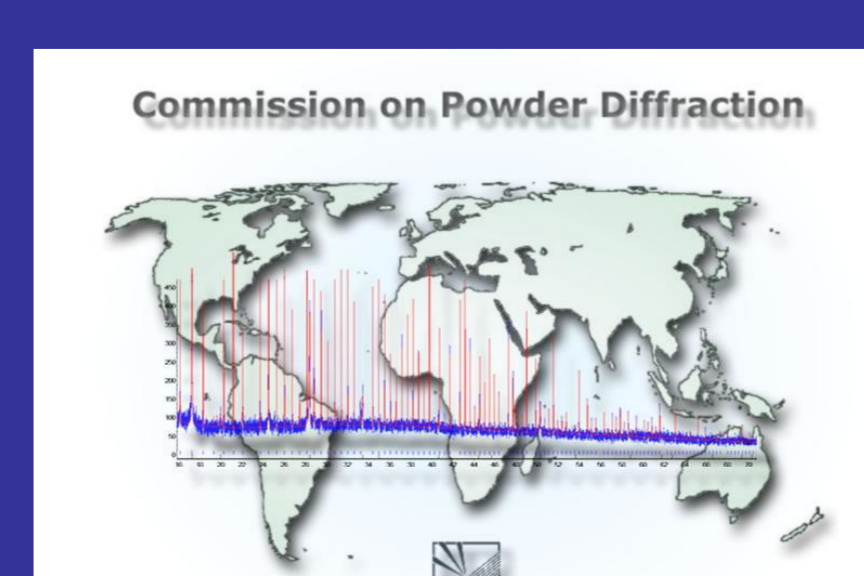
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IUCr Commission on Electron Crystallography

International Workshop on Powder & Electron Crystallography

University of Patras (UPAT), Greece July 2-6, 2013

Conference and Cultural Centre

PROGRAM

Time	July 7 Sunday	July 8 Monday	July 9 Tuesday	July 10 Wednesday	July 11 Thursday	July 12 Friday
8:30-9:20		Direct Methods Giacovazzo	Recent Developments in Precession Electron Diffraction (PED) Nicolopoulos	Synchrotron X-ray Powder Diffraction Fitch	Model refinement in EXPO: wLSQ, RBM, COVMAP Rizzi	Introduction to Protein Powder Diffraction: Overview Von Dreele
9:20-10:00		Direct Methods Giacovazzo	Automated Diffraction Tomography (ADT) Nicolopoulos/ Gemmi	Synchrotron X-ray Powder Diffraction Gozzo	Model refinement in EXPO: wLSQ, RBM, COVMAP Rizzi	Protein Crystallization & Data collection Margiolaki
10:00- 10:30		Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
10:30- 12:30		VLD Phasing Method Giacovazzo	Lab 1 Nicolopoulos/ Gemmi/ Das	Sample preparation & Laboratory X- ray diffraction Beckers	Real Space Methods Rizzi	Structure solution using the MR and SIR/ MIR methods Wright, Margiolaki
12:30- 13:30		Practicals Giacovazzo	Lab 1 Nicolopoulos/ Gemmi/ Stewart/ Das	Unit cell identification Giacovazzo	Lab 2 Cuocci, Rizzi,	Intensity extraction from multiple datasets & Accuracy of protein powder diffraction data Wright
13:30- 15:00		Lunch	Lunch	Lunch	Lunch	Lunch
15:00- 16:00	Registration	Introduction to Precession Electron Diffraction (PED) Gemmi	Lab 1 Nicolopoulos/ Gemmi/ Stewart/ Das	Full pattern decomposition in powders Rizzi	Lab 2 Cuocci, Rizzi	Lab 3 Von Dreele
16:00- 16:30	Registration	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
16:30- 17:30	Registration	Recent Developments in Precession Electron Diffraction (PED) Nicolopoulos	Lab 1 Nicolopoulos/ Gemmi/ Stewart/ Das	Space group identification from powder and electron diffraction data Giacovazzo	Lab 2 Cuocci, Rizzi	Lab 3 Von Dreele
18:00- 22:00	Welcome Ceremony					

Lab 1 : Hands on introduction to the programs ELD, Trice, ADT3D

Lab 2 : Hands on introduction to the programs EXPO

Lab 3 : Hands on introduction to the program GSAS-2