



Crystallography School 2019

Organized by
the Interdepartmental Centre for Crystallography (CrisDi)

The School is aimed at PhD students and graduates without registration fees.

The courses are organized in optional modules. The course enrollment is mandatory. At the end of each module, the students will receive a certificate of attendance (1 credit = 4 hours), subject to a verification.

The language will be English or Italian on request.

The final program and forms for registration are published in the website www.CrisDi.unito.it.

For any further information please refer to P. Benna (piera.benna@unito.it).

FIRST WEEK 27-31 May 2019

BASIC COURSES BC1-BC6

Lecturer: prof. **P. Benna**, University of Torino

BC1. Introduction to Crystallography

1½ CFU (6 hours)

- Crystalline state
- Elements of symmetry
- Point and spatial groups (examples)
- Direct and reciprocal lattice
- International tables.

Lecturer: dr. **A. Agostino**, University of Torino

BC2. Instrumentation for X-Ray Diffraction

1 CFU (4 hours)

- X rays sources
- Filters and monochromator crystals
- Detectors
- Geometries.

Lecturer: dr. **R. Cossio**, University of Torino

BC3. Electron Diffraction

1 CFU (4 hours)

- Electron sources: conventional and FEG
- Magnetic lenses, aberrations and resolution of the electron beam: TEM, STEM, SEM
- Types of electron diffraction: SAED, CBED, EBSD
- Geometry, detectors and new instrumental developments.

Lecturer: prof. **A. Pavese**, University of Torino

BC4. X-Ray Diffraction

1 CFU (4 hours)

- X-rays interaction with matter
- Kinematic theory
- Ewald, Laue, Bragg
- The atomic scattering factor
- The structure factor and diffracted intensity
- The temperature factor.

Lecturer: prof. **M. Milanesio**, University of Piemonte Orientale

BC5. X-Ray Diffraction Methods: Polycrystalline

2½ CFU (10 hours)

- Powder diffraction
 - Principles
 - Experimental design
 - Sample preparation
 - Main instrumental aberrations
 - Peak profile function
- Data analysis
 - Qualitative analysis
 - Data reduction
 - Quantitative analysis.

It is mandatory that students have acquired the knowledge of BC1, BC2 and BC4 courses.

Lecturer: dr. **D. Marabello**, University of Torino

BC6. X-Ray Diffraction Methods: Single Crystal

2½ CFU (10 hours)

- Definition and selection of crystals
- Instrumentation
- Determination of cell parameters
- Data collection
- Structure resolution and refinement
- Critical evaluation of the results
- LAB – PART I
 - Visit to the instrumental laboratory
- LAB – PART II
 - Practice on structure resolution in a computer laboratory.

N° max = 12 students

Attendance at the laboratories will be defined directly by the lecturer in agreement with the students.

It is mandatory that students have acquired the knowledge of BC1, BC2 and BC4 courses.

27-31 May 2019

Aula Diagonale (Via P. Giuria 7, Torino)

*Aula Informatica 3 (To Esposizioni, Corso Massimo D'Azeglio 15, Torino)

	Monday 27 May	Tuesday 28 May	Wednesday 29 May	Thursday 30 May	Friday 31 May
9-10	BC1 - Benna	BC1 - Benna	BC4 - Pavese	BC6 - Marabello	BC6* - Marabello
10-11	BC1 - Benna	BC1 - Benna	BC4 - Pavese	BC6 - Marabello	BC6* - Marabello
11-12	BC2 - Agostino	BC2 - Agostino	BC5 - Milanesio	BC5 - Milanesio	BC6* - Marabello
12-13	BC2 - Agostino	BC2 - Agostino	BC5 - Milanesio	BC5 - Milanesio	BC6* - Marabello
14-15	BC3 - Cossio	BC3 - Cossio	BC6 - Marabello	BC5 - Milanesio	BC5 - Milanesio
15-16	BC3 - Cossio	BC3 - Cossio	BC6 - Marabello	BC5 - Milanesio	BC5 - Milanesio
16-17	BC1 - Benna	BC4 - Pavese	BC6 - Marabello		BC5 - Milanesio
17-18	BC1 - Benna	BC4 - Pavese	BC6 - Marabello		BC5 - Milanesio

SECOND WEEK 3-7 June 2019

SPECIALIZED COURSES SC1-SC6

Lecturer: dr. **G. Di Nardo**, University of Torino

SC1. Structural study of Biological Macromolecules

2 CFU (8 hours)

- Protein crystallization: requirements and strategies
 - Sample preparation
 - Protein crystallization methods and phase diagram
 - Screening of crystallization conditions
 - Optimization of protein crystals: seeding and additional screening
 - Co-crystallization with ligands: soaking
- Protein X rays diffraction • Cryoprotectants and crystals preparation • Sample mounting
- Structural solving methods • Molecular replacement • Anomalous diffraction and isomorphous replacement.

It is mandatory that students have acquired the knowledge of the BC6 course.

Lecturer: prof. **F. Cámara**, University of Milano

SC2. In situ non-ambient conditions by Single Crystal XR Diffraction

2 CFU (8 hours)

- High Temperature • Heating devices, mounting of the crystal and temperature calibration • Effects of temperature
 - Cell parameters and thermal expansion (strain ellipsoid, systematic and predictive equations)
 - Structures (thermal ellipsoid, corrections due to thermal motion)
- High Pressure • Background & technical problems • Cell parameters & equations of state EoS (tools and methods, basic aspects of the EoS, examples) • Structures (tools and methods, examples)
- Examples of distortive phase transitions studied by in-situ SCXRD
 - Expansion of Landau (spontaneous strain, order parameter, coupling elastic energy and order parameters).

It is mandatory that students have acquired the knowledge of the BC5 and BC6 courses.

Lecturer: prof. **A. Ferrari**, University of Torino

SC3. Solid State properties: Modelization

2 CFU (8 hours)

- Introduction to the “CRYSTAL” code
- Dielectric and electronic properties in solids
- Fundamental equations
- Simulation of XRD spectra
- Study cases.

It is mandatory that students have completed the BC1 and BC4 courses.

Lecturer: prof. **R. Giustetto**, University of Torino

SC4. Causes of colour in Minerals

2 CFU (8 hours)

- Crystal Field theory (in octahedron and tetrahedron); Jahn-Teller effect
- Intervalence charge transitions, transitions between valence orbitals and conduction band
- Colour centres; artificial procedures to colour minerals and gems
- Iridescence, luminescence and fluorescence.

Lecturer: dr. **N. Curetti**, University of Torino

SC5. Laboratory of High Pressure experiments - Diamond Anvil Cell (DAC) preparation. 1 CFU (4 hours)

- DAC cell: components and assembly for high pressure experiment
- Use of the standard-crystals for monitoring the internal pressure
- Application of the DAC in X-Ray diffraction experiment.

Lecturer: dr. **F. Bertolotti**, University of Insubria and To.Sca.Lab. (Como)

1 CFU (4 hours)

SC6. The Debye Scattering equation: a Total Scattering approach for characterizing Nanomaterials

- Fundamentals of the Debye Scattering Equation (DSE)
- Data collection and reduction for total scattering experiments
- Characterization of structure, microstructure and morphology of nanocrystals through the DSE
- DSE applications • Modeling of structural defects in nanocrystals: theory and examples • Ligand-induced structural distortions in colloidal semiconductor nanocrystals
- The DebUsSy program suite: an overview
- Tutorial session on the DebUsSy program suite.

It is mandatory that students have completed the BC4 and BC5 courses.

3-7 June 2018

Aula Diagonale (Via P. Giuria 7, Torino)

	Monday 3 June	Tuesday 4 June	Wednesday 5	Thursday 6 June	Friday 7 June
9-10	SC1 Di Nardo	SC1 Di Nardo	SC1 Di Nardo	SC5 Curetti	SC4 Giustetto
10-11	SC1 Di Nardo	SC1 Di Nardo	SC1 Di Nardo	SC5 Curetti	SC4 Giustetto
11-12	SC2 Cámara	SC2 Cámara	SC1 Di Nardo	SC5 Curetti	SC4 Giustetto
12-13	SC2 Cámara	SC2 Cámara	SC1 Di Nardo	SC5 Curetti	SC4 Giustetto
14-15	SC2 Cámara	SC2 Cámara	SC4 Giustetto	SC4 Giustetto	SC6 Bertolotti
15-16	SC2 Cámara	SC2 Cámara	SC4 Giustetto	SC4 Giustetto	SC6 Bertolotti
16-17	SC3 Ferrari	SC3 Ferrari	SC3 Ferrari	SC3 Ferrari	SC6 Bertolotti
17-18	SC3 Ferrari	SC3 Ferrari	SC3 Ferrari	SC3 Ferrari	SC6 Bertolotti

THIRD WEEK 10-14 June 2019

SPECIALIZED COURSES SC7-SC14

Lecturer: dr. **A. Agostino**, University of Torino

SC7. The Rietveld Method

2 CFU (8 hours)

- Basic theory
- Problems with the Rietveld method • Indexing • Peak-shape function (PSF) • Background • Preferred orientation and texture.

It is mandatory that students have completed the BC5 course.

Lecturer: dr. **E. Costa**, University of Torino

SC8. Introduction to Crystal Growth

1½ CFU (6 hours)

- Basic of growth mechanism • Nucleation processes. • Heterogeneous and homogeneous nucleation. • Growth and equilibrium shape. • Interface and roughening.
- Growth technologies • Main growth mechanism. • Melt grown. • Solution grown. • Floating zone growth. • Other methods.
- Characterization of crystals • Crystal defects. • Twins. • Crystal surfaces. • Inclusions and precipitates. • Selected method of characterization. • Etching. • X-ray topography. • Optical microscopy. • Scanning electron microscopy. • Transmission electron microscopy.

Lecturer: dr. **L. Pastoro** University of Torino

SC9. Crystal Growth for beginners

1 CFU (4 hours)

- Ideal crystal vs real crystal
- How to nucleate, grow and modify crystals in lab
- Surfaces and interfaces
- Surface analysis by SPM techniques.

Lecturer: prof. **E. Belluso, S. Capella**, University of Torino

SC10. Use of TEM-EDS for the characterization of natural or synthetic sub-micrometric Inorganic Phases

2 CFU (8 hours)

- Sample preparation
- Data acquisition • Morphology • Electron diffraction • Semi-quantitative composition • Structure
- Refinement of acquired data.

It is mandatory that students have acquired the knowledge of the BC1 and BC4 courses.

Lecturer: prof. **R. Arletti**, University of Torino

SC11. In situ/operando X-Ray Powder Diffraction

1 CFU (4 hours)

- High pressure X-Ray powder diffraction (cell, geometries, conventional and non conventional sources)
- High temperature X-Ray powder diffraction
- In situ/in operando X-ray powder diffraction on porous materials: experiments and data analysis.

It is mandatory that students have completed the BC5 course.

Lecturer: prof. **M. Dapiaggi**, University of Milano

SC12. Pair Distribution function analysis of complex, disorder and amorphous Materials from Total Scattering Data

1 CFU (4 hours)

- Total scattering data: why? How to evaluate the structure-properties relationship of complex and disorder materials
- Basic theoretical needs and experimental setup
- Amorphous 'on the go' ... very short range order
- How to obtain a PDF and how to refine it to a model (practical).

It is mandatory that students have completed BC4 and BC5 courses.

Lecturer: prof. **R. Arletti**, University of Torino

SC13. Inorganic Crystallochemistry

1 CFU (4 hours)

- Basis of the Crystallochemistry
- Compact Packing of Sphere
- Coordination Polyhedra
- Crystalline Structure: examples
- Polymorphism and Isomorphism: examples
- Different kind of Silicates: Chain, Layered, Framework
- Zeolites: structural features and properties.

Lecturer: prof. **S. Bianco, G. Ubertalli, M. Pavese, S. Ronchetti**, Politecnico of Torino

SC14. X-Ray Diffraction applications on Materials Study

2 CFU (8 hours)

- Synthesis, characterization and application of nanostructured oxides
- Stress analysis in metallic materials by X-ray diffraction
- Microdiffraction technique
- Non ambient X-ray diffraction: a technique to understand the influence of temperature, atmosphere or pressure on materials.

It is mandatory that students have completed the BC5 course.

10-14 June 2019

Aula Diagonale (Via P. Giuria 7, Torino)

*Aula Informatica 3 (To Esposizioni, Corso Massimo D'Azeglio 15, Torino)

	Monday 10 June	Tuesday 11 June	Wednesday 12 June	Thursday 13 June		Friday 14 June
				DIP CHIMICA	POLITECNICO	
9-10	SC7 Agostino	SC7 Agostino	SC7* Agostino	SC12 Dapiaggi	SC14 Ronchetti et al	SC10 Belluso/Capella
10-11	SC7 Agostino	SC7 Agostino	SC7* Agostino	SC12 Dapiaggi	SC14 Ronchetti et al	SC10 Belluso/Capella
11-12	SC8 Costa	SC8 Costa	SC7* Agostino	SC12 Dapiaggi	SC14 Ronchetti et al	SC8 Costa
12-13	SC8 Costa	SC8 Costa	SC7* Agostino	SC12 Dapiaggi	SC14 Ronchetti et al	SC8 Costa
14-15	SC9 Pastero	SC9 Pastero	SC11* Arletti	SC13 Arletti	SC14 Ronchetti et al	SC10 Belluso/Capella
15-16	SC9 Pastero	SC9 Pastero	SC11* Arletti	SC13 Arletti	SC14 Ronchetti et al	SC10 Belluso/Capella
16-17	SC10 Belluso	SC10 Belluso	SC11* Arletti	SC13 Arletti	SC14 Ronchetti et al	
17-18	SC10 Belluso	SC10 Belluso	SC11* Arletti	SC13 Arletti	SC14 Ronchetti et al	