



«ETTORE MAJORANA» FOUNDATION AND CENTRE FOR SCIENTIFIC CULTURE  
TO PAY A PERMANENT TRIBUTE TO ARCHIMEDES AND GALILEO GALILEI, FOUNDERS OF MODERN SCIENCE  
AND TO ENRICO FERMI, THE "ITALIAN NAVIGATOR", FATHER OF THE WEAK FORCES



# INTERNATIONAL SCHOOL OF CRYSTALLOGRAPHY

## 57th Course: DIFFUSE SCATTERING: THE CRYSTALLOGRAPHY OF DYNAMICS, DEFECTS AND DISORDER

ERICE-SICILY: 3 – 11 JUNE 2022

Sponsored by the: • European Crystallographic Association • International Union of Crystallography •  
• Italian Ministry of Education, University and Scientific Research • Sicilian Regional Government

### PROGRAMME AND LECTURERS

#### *Protein correlated motions*

• N. ANDO, Cornell University, NY, US

#### *Biological diffuse scattering at XFELs*

• K. ÄYDYER, MPSD Hamburg, DE

#### *The pair distribution function*

• S. BILLINGE, Columbia University, NY, US

#### *Inelastic scattering*

• A. BOSAK, ESRF, Grenoble, FR

#### *Monte Carlo modelling*

• H.B. BURGI, University of Bern, CH

#### *Single-crystal neutron diffuse scattering*

• S. CAPELLI, ISIS, UK

#### *In situ/in operando studies*

• K. CHAPMAN, Stony Brook, NY, US

#### *Temperature and dynamics in structural biology*

• J. FRASER, UCSF, CA, US

#### *X-ray diffraction theory*

• H. GINN, University of Hamburg, DE

#### *Diffuse scattering in materials chemistry*

• A. GOODWIN, Oxford University, UK

#### *The Debye equation*

• A. GUAGLIARDI, IC-CNR, Como, IT

#### *Time-resolved macromolecular crystallography*

• D. HEKSTRA, Harvard University, MA, US

#### *Nanomaterials*

• K. JENSEN, University of Copenhagen, DK

#### *Historical context of diffuse scattering*

• D. KEEN, ISIS, UK

#### *Lattice dynamics in biological diffuse scattering*

• S. MEISBURGER, Cornell University, NY, US

#### *DISCUS*

• R. NEDER, University of Erlangen, DE

#### *Diffuse scattering in materials physics*

• R. OSBORN, ANL, US

#### *Unconventional magnetism*

• J. PADDISON, ORNL, US

#### *Models of protein diffuse scattering*

• A. PECK, Stanford SLAC, US

#### *3D- $\Delta$ PDF methods*

• A. SIMONOV, ETH Zürich, CH

#### *High pressure and total scattering*

• M. TUCKER, ORNL, US

#### *MD simulations of biological diffuse scattering*

• M. WALL, LANL, US

#### *Analysis of MD simulations of protein crystals.*

• D.C. WYCH, LANL, US

### PURPOSE OF THE COURSE

Periodic order is the sine qua non of crystallography. Yet sometimes it is the departure from order that is crucial for material function. Proteins, frustrated magnets, photovoltaics, battery materials, high-temperature superconductors — there are many examples of important systems where disorder of one sort or another plays a pivotal role. Crystallographically, the signature of disorder is the existence of a diffuse component to the scattering function, usually orders of magnitude weaker than the conventional Bragg scattering. The advent of intense radiation sources, the development of revolutionary detector technologies, and the ready availability of high-performance computing have collectively transformed our ability to measure and interpret diffuse scattering from disordered crystals. As a result, scientists across many disciplines — from biochemistry to condensed-matter physics — are discovering all sorts of new types of disorder and importantly, all sorts of new ways in which disorder is critical for function. This Course will cover the background necessary to measure and interpret diffuse scattering from disordered crystals. Its contents span the theory of diffraction and diffuse scattering, the practicalities of its measurement, and the many different approaches taken to its interpretation. The programme is loosely split into two strands — one with a focus on materials chemistry & physics and the other concerned mostly with protein dynamics. Collectively, the course will cover the various origins of diffuse scattering (e.g. dynamics, compositional/displacive disorder, magnetic disorder), and its form in both single-crystal and powder samples. There will be extensive discussion of real-space interpretations, including the well-known pair distribution function (PDF) and its variants (e.g. 3D- $\Delta$ PDF). These lectures will draw on and highlight key scientific discoveries from the recent literature. In parallel to the lecture course, the course will offer a broad selection of tutorials and workshops that will cover many of the key analysis approaches: such as molecular dynamics, Monte Carlo simulations, the Debye equation, small-box and big-box atomistic modelling.

### APPLICATIONS

Interested candidates should register by 13rd December 2021 using the form available at the URL <http://erice2022.azuleon.org> or by writing to the Executive Secretary of the International School of Crystallography:

Dr. Annalisa Guerri

University of Florence

50019 Sesto Fiorentino, Italy

Tel: +39.055.4573429

email: [annalisa.guerri@unifi.it](mailto:annalisa.guerri@unifi.it)

Please include the following information in your application: i) Your full name(s), age, gender, citizenship; ii) Your postal address, phone, fax, electronic mail; iii) Your present academic position and scientific interests; iv) The title or abstract of a scientific contribution to the poster session(s) which might be included in the programme. Applicants may be able to apply for partial financial support. Please visit [www.crystallalice.org](http://www.crystallalice.org) to view the full eligibility criteria. Young researchers should include in their application a list of no more than five scientific publications that they have authored, and a letter of recommendation from their supervisor or from a senior scientist, that justifies any support that the researcher requests. In order to reflect the multi-disciplinary nature of the Course, priority will be given to applicants who have an appropriate scientific discipline, a good publication rate and a strong correspondence between their current research interest and the topics covered by the School.

### POETIC TOUCH

According to legend, Erice, son of Venus and Neptune, founded a small town on top of a mountain (750 metres above sea level) more than three thousand years ago. The founder of modern history — i.e. the recording of events in a methodic and chronological sequence as they really happened without reference to mythical causes — the great Thucydides (~500 B.C.), writing about events connected with the conquest of Troy (1183 B.C.) said: «After the fall of Troy some Trojans on their escape from the Achaean arrived in Sicily by boat and as they settled near the border with the Sicilians all together they were named Elymi: their towns were Segesta and Erice.»

This inspired Virgil to describe the arrival of the Trojan royal family in Erice and the burial of Anchises, by his son Aeneas, on the coast below Erice. Homer (~1000 B.C.), Theocritus (~300 B.C.), Polybius (~200 B.C.), Virgil (~50 B.C.), Horace (~20 B.C.), and others have celebrated this magnificent spot in Sicily in their poems. During seven centuries (XIII-XIX) the town of Erice was under the leadership of a local oligarchy, whose wisdom assured a long period of cultural development and economic prosperity which in turn gave rise to the many churches, monasteries and private palaces which you see today.

In Erice you can admire the Castle of Venus, the Cyclopean Walls (~800 B.C.) and the Gothic Cathedral (~1300 A.D.). Erice is at present a mixture of ancient and medieval architecture. Other masterpieces of ancient civilization are to be found in the neighbourhood: at Motya (Phoenician), Segesta (Elymian), and Selinunte (Greek). On the Aegadian Islands — theatre of the decisive naval battle of the first Punic War (264-241 B.C.) — suggestive neolithic and paleolithic vestiges are still visible: the grottoes of Favignana, the carvings and murals of Levanzo.

Splendid beaches are to be found at San Vito Lo Capo, Scopello, and Cornino, and a wild and rocky coast around Monte Cofano: all at less than one hour's drive from Erice.

More information about the «Ettore Majorana» Foundation and Centre for Scientific Culture can be found on the WWW at the following address:  
<http://www.ccsem.infn.it>

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### PLEASE NOTE

Participants must arrive in Erice no later than 8 p.m. on 3rd June 2022.