



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



# INTERNATIONAL SCHOOL OF CRYSTALLOGRAPHY

## 49th Course:

### HIGH-PRESSURE CRYSTALLOGRAPHY: STATUS ARTIS AND EMERGING OPPORTUNITIES IN CBRN DEFENCE

ERICE-SICILY: 27 MAY – 5 JUNE 2016

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



#### PROGRAMME AND LECTURERS

##### Data analysis

##### Phase transitions in minerals

• R.J. ANGEL, University of Padova, IT

##### Structure and dynamics of ice and ice clathrates

• L.E. BOVE, École Polytechnique Fédérale de Lausanne, CH, and Université Pierre et Marie Curie, Paris, FR

##### Biological systems and high-pressure SAXS

• N.J. BROOKS, Imperial College London, UK

##### Pair distribution function analysis

##### MOFs and other framework materials

• K.W. CHAPMAN, APS, Argonne National Laboratory, US

##### Dynamic compression

• J.H. EGGERT, Lawrence Livermore National Laboratory, CA, US

##### Pharmaceutical drug molecules

• F.P.A. FABBIANI, Georg-August Universität Göttingen, DE

##### Neutron diffraction

##### Instrumental innovations at neutron sources

• M. GUTHRIE, European Spallation Source, Lund, SE

##### Multianvil techniques and their application in Earth and materials sciences

• T. IRIFUNE, Ehime University, Matsuyama, Ehime, JP

##### Mössbauer spectroscopy

##### Inelastic scattering

• J.M. JACKSON, California Institute of Technology, Pasadena, CA, US

##### In situ high-pressure crystallisation

• A. KATRUSIAK, Adam Mickiewicz University, Poznan, PL

##### New materials under extreme environments

##### Advances in instrumentation at photon sources

• W.L. MAO, Stanford University and SLAC, Menlo Park, CA, US

##### Pressure-induced amorphisation

• D. MACHON, Université Claude Bernard, Lyon1, FR

##### Synchrotron and neutron studies in planetary science

• H.E. MAYNARD-CASELY, ANSTO, Lucas Heights, AU

##### Complex structures of the elements

• M.I. McMAHON, The University of Edinburgh, UK

##### Techniques for materials discovery and optimisation using high-pressure synthesis

• J.B. PARISE, Stony Brook University, New York, NY, US

##### Understanding phase stability: intermolecular interactions in molecular crystals

##### Single-molecule magnets

• S. PARSONS, The University of Edinburgh, UK

##### Structure and magnetism in compressed matter

• S. PASCARELLI, ESRF, Grenoble, FR

##### Crystal structure prediction

• C.J. PICKARD, University College London, UK

##### Liquids and glasses

• C. SANLOUP, The University of Edinburgh, UK, and Université Pierre et Marie Curie, Paris, FR

##### Materials' properties at extreme pressure/temperature conditions: theory and experiments

• B. WINKLER, Johann Wolfgang Goethe-Universität Frankfurt am Main, DE

#### PURPOSE OF THE COURSE

Since the award of the Nobel Prize in Physics to Percy W. Bridgman in 1946 "for the invention of an apparatus to produce extremely high pressures, and for the discoveries he made therewith in the field of high pressure physics", tremendous advances have been made in the field of high-pressure crystallography. Bridgman's use of novel technical approaches to drive discovery finds an echo in modern high-pressure crystallography: New experimental and theoretical approaches allow us to address fundamental scientific questions from disciplines such as Physics, Chemistry, Biology, Geosciences and Materials Science. An ever expanding use of high pressure - from the very modest pressure required to induce the denaturation of proteins and modify intermolecular interactions, through the higher pressures required to synthesise new materials for technological application, to the ultra-high pressures required to radically alter the chemical physical properties of simple elements and materials or recreate the conditions found in Earth's and other planets' interior - is making it a versatile and central tool in condensed matter science.

The objective of this course is to educate young researchers in the interdisciplinary aspects of high-pressure crystallography research and to inspire the next generation of high-pressure scientists to leave their own stamp on the field. Fundamental topics covered in the course include experimental techniques for pressure generation, X-ray and neutron diffraction on single crystal and powder materials, comparative structural studies as well as combined high-temperature and low-temperature experiments. These will be demonstrated through examples of different chemical and structural complexity, including minerals, elements, molecular crystals, ices and biomolecules. Specialised and frontiers high-pressure research topics will include computational crystallography, dynamic compression, characterisation of liquids and glasses and pair distribution function analysis. The course will be rounded up by illustrating the use of high-pressure as a means to study and access new materials for industrial application such as pharmaceuticals, energy storage, magnetic and ultra-hard materials.

Lectures will be complemented by demonstration and workshop sessions. The course will provide a platform for young and senior scientists to interact and identify as well as discuss new challenges in this rapidly evolving and vibrant research area.

#### HOW TO APPLY

Interested candidates should register by 30th November 2015 using the form available at the URL <http://erice2016.azuleon.org> or by writing to the Executive Secretary of the International School of Crystallography:

- Dr. Annalisa Guerri  
Department of Chemistry  
University of Florence  
Via della Lastruccia, 3  
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:

- Your full name(s), age, gender, citizenship;
- Your postal address, phone, fax, electronic mail;
- Your present academic position and scientific interests;
- The title or abstract of a scientific contribution to the poster session(s) which might be included in the programme.

M. GUTHRIE – J.B. PARISE  
DIRECTORS OF THE COURSE

T.L. BLUNDELL  
DIRECTOR OF THE SCHOOL

A. ZICHICHI  
EMFCSC PRESIDENT AND DIRECTOR OF THE CENTRE

#### 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 Achaei 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 International School of Crystallography can be found on the WWW at the following address:  
<http://www.crystalleric.org>

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>

#### PLEASE NOTE

Participants must arrive in Erice no later than 8 p.m. on 27<sup>th</sup> May 2016.

Applicants may be able to apply for partial financial support. Please visit [www.crystalleric.org](http://www.crystalleric.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.