«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

52nd Course: QUANTUM CRYSTALLOGRAPHY

ERICE-SICILY: 1 – 10 JUNE 2018

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

PROGRAMME AND LECTURERS

X-ray constrained wave functions
• D. JAYATILAKA, University of Western Australia, AU

Atomic polarizabilities and dielectric properties of crystals
• P. MACCHI, University of Bern, CH

Crystal orbital theoretical calculations
• B. CIVALLERI, University of Turin, IT

Electron charge and spin density
• N. CLAISER, University of Lorraine, FR

Chemical Bonding in solids
• J. CONTRERAS, Sorbonne University, FR

Electron charge and spin density
• M. DEUTSCHE, University of Lorraine, FR

X-ray constrained wave functions
• B. DITTRICH, University of Düsseldorf, DE

Femto-second X-ray diffraction
• T. ELSAESSER, Max Born Institute, Berlin, DE

Properties from periodic wave functions
• A. ERBA, University of Turin, IT

X-ray constrained molecular orbitals
• A. GENONI, CNRS, FR

Calculations of electronic structures in crystals
• P. GIANNOZZI, University of Udine, IT

Experimental atomic forces in crystals
• F. GIESSIBL, University of Regensburg, DE

Electron density in momentum space
• J. M. GILLET, Ecole Centrale Paris, FR

Hirshfeld atom refinement
• S. GRABOWSKI, University of Bremen, DE

Charge density in biomolecules
• B. GUILLOT, University of Lorraine, FR

Dynamics in crystals
• A. MADSEN, University of Copenhagen, DK

Quantum crystallography
• L. MASSA, City University of New York, NY, US

Quantum chemistry in protein crystals
• K. MERZ, Michigan State University, MI, US

Electron density from electron diffraction
• P. NAKASHIMA, Monash University, AU

Dispersion corrected DFT methods for solids
• M. NEUMANN, Avangarde, DE

Accurate X-ray diffraction measurements
• J. OVERGAARD, University of Aarhus, DK

Experimental quantum chemistry
• M. RAHM, Chalmers University, SE

Quantum crystallography and crystal engineering
• M. SPACKMAN, University of Western Australia, AU

Bonding and properties in metal organic solids
• W. SCHERER, University of Augsburg, DE

QM/MM approaches in bioinorganic chemistry
• U. RYDE, Lund University, SE

PURPOSE OF THE COURSE

This is the inaugural School on Quantum Crystallography at Erice. Quantum Crystallography refers to the combination of crystallographic information from diffraction or other scattering techniques with quantum mechanical theory. It is also an extension of quantum chemistry to periodic systems.

The School attempts to give a snapshot of this evolving field, complete with workshops demonstrating state-of-the art software. Topics will include: the beginnings of the Quantum Crystallography in the measurement of the electron charge or spin density; the Hohenberg-Kohn theorem and the importance of the X-ray diffraction experiment; multipole-based models for the charge density; polarizable-density models; momentum based experiments and orbital density expansions; joint refinement of charge, spin, and momentum density.

APPLICATION

Interested candidates should register by 30th November 2017 using the form available at the URL **http://erice2018.azuleon.org** or by writing to the Executive Secretary of the International School of Crystallography:

Dr. Annalisa Guerri
University of Florence – Via della Lastruccia, 3 – 50019 Sesto Fiorentino, IT
Tel: +39.055.4573429 – email: *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.crystalerice. 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.

PLEASE NOTE

Participants must arrive in Erice no later than 8 p.m. on 1st June 2018.

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 Sicanians 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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http://www.crystalerice.org

P. MACCHI - D. JAYATILAKA
DIRECTORS OF THE COURSE

T.L. BLUNDELL
DIRECTOR OF THE SCHOOL

A. ZICHICHI
EMFCSC PRESIDENT AND DIRECTOR OF THE CENTRE