



«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 LIQUID CRYSTALS

24th Course: *EXTENDED MODEL OF ORGANIC SEMICONDUCTORS* ERICE-SICILY: 1 – 7 OCTOBER 2018

Sponsored by the: • Italian Ministry of Education, University and Scientific Research • Sicilian Regional Government

PROGRAMME AND LECTURERS

Charge-transport in carbon-based materials: A microscopic view

• D. BELJONNE, University of Mons, Mons, BE

Molecular-scale modeling of charge transport and excitonics in organic devices

• P. BOBBERT, Technische Universiteit Eindhoven, Eindhoven, NL

Applications of wavelet-based density functional theory

• T. DEUTSCH, Institut Nanosciences et Cryogénie Grenoble (CEA), Grenoble, FR

Electronic and optical properties of organic systems with embedded many-body perturbation theory

• I. DUCHEMIN, Institut Nanosciences et Cryogénie Grenoble (CEA), Grenoble, FR

Doping-induced phenomena in organic semiconductors: insights from kMC simulations

• A. FEDAI, Karlsruhe Institute of Technology, Karlsruhe, DE

Design principles for charge carrier mobility and anisotropic orientation of organic semiconductors

• P. FRIEDERICH, Karlsruhe Institute of Technology, Karlsruhe, DE

Organic solid state emitters by design

• J. GIERSCHE, Madrid Institute for Advanced Studies, Madrid, ES

Efficient exciton diffusion in a donor-acceptor conjugated dye for solar cells applications: Theoretical insights

• G. LONDI, University of Mons, Mons, BE

Device level design for the microelectronic industry

• A. NEJIM, Silvaco Europe Ltd, St. Ives, UK

Performing multiscale OLED simulations using industry-ready software

• T. NEUMANN, Nanomatch GmbH, Eggenstein-Leopoldshafen, DE

Dissecting the nature of the relevant singlet and triplet excited states in TADF molecular materials

• Y. OLIVIER, University of Mons, Mons, BE

Ab initio-based approach to the density of states of doped organic semiconductors

Theoretical prediction of the density of states of n-doped organic films and comparison to experiments

• F. ORTMANN, Technische Universität Dresden, Dresden, DE

Impact of contact resistance on the integration of organic thin film transistors

• C. ROLIN, IMEC, Leuven, BE

Atomistic and coarse-grained modelling and simulation

• O.M. ROSCIONI • L. QUERCIAGROSSA • M. RICCI, Università di Bologna, Bologna, IT

OFET and charge transport in small molecule organic semiconductors

Structure-property relationships in thienosiloles for improved charge transport

• G. SCHWEICHER, University of Cambridge, Cambridge, UK

Simulating organic semiconductors: the challenge of amorphous materials

• A. SMITH, University of Bath, Bath, UK

Modelling charge transport in organic semiconductors at the mesoscale

• I. THOMPSON, University of Bath, Bath, UK

Multiscale modelling and molecular design of organic semiconductor materials

• W. WENZEL, Karlsruhe Institute of Technology, Karlsruhe, DE

100% Organic: Understanding organic electronics from molecules to devices

• A. WALKER, University of Bath, Bath, UK

Injection, transport, and recombination of charges in organic-semiconductor diodes

• G.A.H. WETZEL, Max Planck Institute, Mainz, DE

FlexEnable's OTFT technology and its applications

• B. YAGLIOGLU, FlexEnable Limited Ltd, Cambridge, UK

Modeling morphologies by molecular dynamics

• C. ZANNONI, University of Bologna, Bologna, IT

PURPOSE OF THE WORKSHOP

The aim of the Course is to provide an overview of the state of the art of the European project EXTMO which has as main objective the creation of materials model and the related user friendly code that will focus on charge transport in doped organic semiconductors. Its aims are: to reduce the time to market of (a) multilayer organic light emitting devices, OLEDs, with predictable efficiencies and long lifetimes (b) organic thin film transistors and circuits with fast operation to reduce production costs of organic devices by enabling a fully solution processed technology. Development costs and times will be lowered by identifying dopants that provide good device performance, reducing the number of dopant molecules that need to be synthesized and the materials required for trial devices, to reduce design costs at circuit level through an integrated model linking molecular design to circuit operation. Screening imposes the following requirements from the model: 1) An improved understanding of dopant/host interactions at the molecular level. Doping efficiencies need to be increased to give better conducting materials. For OLEDs, dopants should not absorb visible light that lowers output nor ultraviolet light that can cause degradation. 2) An ability to interpret experimental measurements used to identify the best dopants. 3) The possibility of designing dopants that are cheap and (photo)chemically robust and whose synthesis results in fewer unwanted impurities, and that are less prone to clustering. The EXTMO model is developed at the mesoscopic level with embedded atomistic level electronic structure and molecular packing calculations. Modules at the continuum and circuit levels are an integral part of the model. It will be validated by measurements on single and multiple layer devices and circuits and exploited by 2 industrial end users and 2 software vendors. US input is provided by an advisory council of 3 groups whose expertise complements that of the partners.

APPLICATIONS

Persons wishing to attend the Course should apply writing to:
Paolo PASINI, INFN of Bologna, Bologna, Italy
E-mail: Paolo.Pasini@bo.infn.it

PLEASE NOTE

Participants are expected to arrive in Erice on October 1, no later than 5 p.m.

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 Anchise, by his son Enea, 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 other activities of the
«ETTORE MAJORANA» FOUNDATION AND CENTRE FOR SCIENTIFIC CULTURE
can be found on the WWW at the following address:
<http://www.ccsem.infn.it>