



# Math/Chem/Comp 2015

## 27<sup>th</sup> MC<sup>2</sup> Conference

### The 2<sup>nd</sup> Circular

The 27<sup>th</sup> International Course and Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences (Math/Chem/Comp, MC<sup>2</sup>-27) will be held on June 12–19, 2015, in Dubrovnik, Croatia under the joint auspices of the Inter-University Center, Dubrovnik, Croatia, the University of Zagreb, the University of Split, and the Rudjer Bošković Institute, Zagreb, Croatia.

**Conference website:** <http://www.pmf.unizg.hr/chem/mathchemcomp>

#### CONFERENCE BOARD

**Director:** Hrvoj Vančik, Professor of Chemistry, University of Zagreb, Croatia

**Co-director:** Jerzy Cioslowski, Professor of Physics, University of Szczecin, Poland

#### SCIENTIFIC COMMITTEE

Vincenzo Aquilanti (University of Perugia, Italy), Attila Czaszar (Eötvös University, Budapest, Hungary), Tomica Hrenar (University of Zagreb, Croatia), Roland Mitrić (University of Würzburg, Germany), Dejan Plavšić (Ruđer Bošković Institute, Zagreb, Croatia), Andreas Savin (UPMC Sorbone University, Paris, France), Miguel Sola (University of Girona, Spain), Peter Stadler (University of Leipzig, Germany), Peter Surjan (Eötvös University, Budapest, Hungary), Jesus Ugalde (Euskal Herriko University, Euskadi, Spain), Dražen Vikić-Topić (Ruđer Bošković Institute, Zagreb, Croatia), Damir Vukičević (University of Split, Croatia)

#### HONORARY COMMITTEE

Aleksandru Balaban, Mircea Diudea, Ivan Gutman, Edward Kirby, Milan Randić, Nenad Trinajstić, Tomislav Živković

#### VENUE

MC<sup>2</sup>-27 meeting will be held in Dubrovnik on 12–19 June, 2015. Dubrovnik is situated on Adriatic Coast in the southern part of the Republic of Croatia and, in recognition of its beauty,

has been designated by UNESCO as a world heritage site. The venue of the meeting will be the Inter-University Centre (IUC) located at don Frana Bulica 4 (in the vicinity of the western gate [Vrata od Pila]) of the Old City.

## CONFERENCE SCOPE AND SCIENTIFIC PROGRAM

Since 1986, the Math/Chem/Comp meetings have been bringing together researchers working on diverse subjects spanning mathematics, computer science, and chemistry. In continuation of this tradition, presentations concerning all aspects of current research on computer modeling, combinatorics, graph theory, and topology applied to any area of chemistry, physics, material and life sciences will be welcomed. The conference program will include invited plenary and special lectures workshops and posters. In particular, the MC<sup>2</sup>-27 meeting will revolve around the following topics:

1. Mathematical chemistry and chemical graph theory (in memory of Professor Ante Graovac);

### **Plenary Lecture**

Dr Damir Vukičević (*University of Split*): **Mathematical research of molecular descriptors**

2. Mathematical methods and computational algorithms in modeling of atoms, molecules, and chemical processes;

### **Plenary Lecture**

Prof. Tomica Hrenar (*University of Zagreb*): **Computational Algorithms in Conformational Analysis of Cyclic and Non-cyclic Molecules**

3. Molecular modeling in practice (including molecular dynamics and aggregation);

### **Plenary Lecture**

Prof. Ricardo Mata (*Georg-August-Universität Göttingen*): **Sampling strategies for QM/MM calculations in condensed phase**

### **Special Lecture**

Dr. Jens Petersen (*Julius-Maximilians Universität Würzburg*): **Simulation and control of light-induced dynamics in complex molecular systems**

4. Discussion about the future of mathematical modeling in chemistry.

## **Plenary Lecture**

Prof. Hrvoj Vančik (*University of Zagreb*)

## **Workshops**

Prof. Zlatko Mihalić (*University of Zagreb*): **Course on Molecular Modeling**

## **Poster Sessions**

### **REGISTRATION AND ABSTRACT**

Participants may register and submit abstracts by e-mail to the director of the conference at the address:

[vancik@chem.pmf.hr](mailto:vancik@chem.pmf.hr)

### **Registration submission deadline: April 15, 2015**

The abstract template will be available on the conference website.

### **Abstract submission deadline: May 15, 2015**

**Abstracts in other formats will not be accepted.**

### **POSTERS**

The recommended dimensions of the posters are 90×120 cm (16.5"×22"). All posters to be presented should include a conference logo (available on the conference website), concise title, names and complete addresses of authors with indication of the author presenting the poster.

### **PROCEEDINGS**

The papers presented at the MC<sup>2</sup>-27 meeting will be published as a special issue of *Croatica Chemica Acta*.

All contributions will be refereed. The participants are encouraged to submit their manuscripts before the meeting or at the latest upon arrival in Dubrovnik. Those unable to attend are invited to send their manuscripts to the director of the conference.

### **REGISTRATION FEE**

The conference registration fee includes the following:

- admission to all scientific sessions
- conference materials
- coffee or juice at breaks
- welcome drink
- guided sightseeing city tour
- IUC reception party

### **Registration fee**

Before April 15, 2014: 180.00 € (80.00 € for students\*) + 25% VAT.

After April 15, 2014: 200.00 € (100.00 € for students\*) + 25% VAT.

Accompanying persons: 100.00 € + 25% VAT.

\*Conference participants without Ph. D. degrees. A letter from the undergraduate mentor or the Ph.D. advisor is required.

### **Payment**

Bank transfer to

BANK NAME: **Zagrebačka banka d.d.**

BANK ADDRESS: Paromlinska 2, 10000 Zagreb, Croatia

IBAN: **HR582360001101522208**

SWIFT/BIC CODE: **ZABHR2X**

ACCOUNT HOLDER: Sveučilište u Zagrebu Prirodoslovno-matematički fakultet, Horvatovac 102A, 10000 Zagreb

ACCOUNT NAME: **Math.Chem.Comp.**

**Name of the participant is required**

### **THE DIRECTOR**

All correspondence concerning the meeting should be addressed to:

**Prof. Hrvoj Vančik**

Department of Chemistry, Faculty of Sciences and Mathematics,

University of Zagreb

Horvatovac 102A, 10000 Zagreb, Croatia

phone: 385 1 4606 400; fax: 385 1 4606 401

e-mail: [vancik@chem.pmf.hr](mailto:vancik@chem.pmf.hr)

## **ACCOMMODATION AND TRANSPORTATION**

The participants will be accommodated in hotels "Lero" and "R". These hotels are within walking distance from the conference site. The participants are asked to make their hotel reservations directly by applying to:

**Hotel "LERO"** (AX, EC/MC, DC, VISA)

phone: +385 20 332 022 fax: +385 20 332 123

e-mail: [luka@hotel-lero.hr](mailto:luka@hotel-lero.hr)

website: [www.hotel-lero.hr](http://www.hotel-lero.hr)

or

**Hotel "R"**

phone: +385 20 333 200 fax: +385 20 333 208

e-mail: [helpdesk@hotel-r.hr](mailto:helpdesk@hotel-r.hr)

website: [www.hotel-r.hr](http://www.hotel-r.hr)

The participants are urged to make reservations as soon as possible as the number of rooms is limited and Dubrovnik is a popular tourist destination. Further information regarding reservations of accommodation and other tourist matters can be obtained by e-mailing to [edrakulic@chem.pmf.hr](mailto:edrakulic@chem.pmf.hr).

The city of Dubrovnik can be reached by air from Zagreb and European cities, by bus coaches from Zagreb, Rijeka and Split, by boat from the ports of Rijeka and Split, or by boat from Italy.

**The participants are responsible for booking of accommodation and transportation. The conference organizers cannot assume any responsibility for these matters.**