# Math/Chem/Comp 2016 28<sup>th</sup> MC<sup>2</sup> Conference The 3<sup>rd</sup> Circular

The 28<sup>th</sup> International Course and Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences (Math/Chem/Comp, MC<sup>2</sup>-28) will be held on **June 20–25, 2016, 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.

#### SPONSORED BY













Centar za NMR

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

# VENUE

MC<sup>2</sup>-28 will be held in Dubrovnik on 20–26 June, 2016. 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>-28 meeting will revolve around the following topics:

1. Mathematical chemistry and chemical graph theory;

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

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

4. Molecular logics gates.

#### **SPECIAL EVENT**

The first session of the conference will be dedicated to the **80<sup>th</sup> birthday of Professor Nenad Trinajstić**, one of the establishers of chemical graph theory and MathChemComp conference series.

#### MATH/CHEM/COMP NMR SUB-CONFERENCE

## **NMR: From Theory to Biomolecules**

#### **Organization committee**

**Predrag Novak-chair,** University of Zagreb, Faculty of Science, Department of Chemistry, **Dražen Vikić Topić,** Ruđer Bošković Institute, University of Rijeka, **Jelena Parlov Vuković,** INA-Industrija nafte d.d., Refining & marketing business division, Product development department, Lovinčićeva bb, 10002 Zagreb, Croatia

#### **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

#### **Conference website:**

http://www.pmf.unizg.hr/chem/mathchemcomp

Registration deadline: April 15, 2016.

Abstract submission deadline: May 15, 2016.

The abstract template will be available on the conference website. Abstracts in other formats will not be accepted.

## POSTERS

The recommended dimensions of the posters are  $90 \times 120$  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  $MC^2$ -28 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.

## WORKSHOP: AB INITIO MOLECULAR DYNAMICS

## **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, 2016: 180.00 € (80.00 € for students\*) + 25% VAT.

After April 15, 2016: 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 ADRESS: Paromlinska 2, 10000 Zagreb, Croatia

IBAN: HR5823600001101522208 SWIFT/BIC CODE: ZABAHR2X

ACCOUNT HOLDER: Sveučilište u Zagrebu Prirodoslovnomatematički fakultet, Horvatovac 102A, 10000 Zagreb

ACCOUNT NAME: Math.Chem.Comp.

Name of the participant is required!

#### 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: <u>vancik@chem.pmf.hr</u>

#### ACCOMMODATION AND TRANSPORTATION

Other accomodation info available at:

http://www.iuc.hr/private-accomodation.php http://www.iuc.hr/hotels.php

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 in-formation regarding reservations of accommodation and other tourist matters can be obtained by e-mailing to Ms. Danijela Štrman <u>danijela.strman@gulliver.hr</u> or to <u>edrakulic@chem.pmf.hr</u>.

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.