# Math/Chem/Comp 2019

#### 31st MC<sup>2</sup> Conference

The 31<sup>st</sup> International Course and Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences (Math/Chem/Comp, MC<sup>2</sup>-31), organized under the joint auspices of the Inter-University Centre, Dubrovnik, Croatia, and the University of Zagreb (Department of Chemistry, Faculty of Science), will be held on June 10–14, 2019 in Dubrovnik (Croatia).

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

#### **CONFERENCE BOARD**

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

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

#### **SCIENTIFIC COMMITTEE**

Dragan Amić (Josip Juraj Strossmayer University of Osijek, Croatia), Vincenzo Aquilanti (University of Perugia, Italy), Attila G. Császár (Eötvös University, Budapest, Hungary), Tomica Hrenar (University of Zagreb, Croatia), Bono Lučić (Ruđer Bošković Institute, 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), Péter Surján (Eötvös Loránd University, Budapest, Hungary), Jesus Ugalde (Euskal Herriko University, Euskadi, Spain), Dražen Vikić-Topić (University of Rijeka, Ruđer Bošković Institute, Zagreb, Croatia),

#### HONORARY COMMITTEE

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

#### **VENUE**

MC<sup>2</sup>-31 will be held in Dubrovnik on 10–14 June, 2019. 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>-31 meeting will revolve around the following topics:

- 1. Mathematical methods and computational algorithms in modeling of atoms, molecules, and chemical processes;
- 2. Mathematical chemistry and chemical graph theory;
- 3. Molecular modeling in practice (including molecular dynamics and aggregation);
- 4. Chemical experiments, industrial processes, and mathematical interpretation

#### SCIENTIFIC PROGRAM

The conference program will include invited lectures, contributed oral presentations, and posters.

Special section in memory to Professor Edward Kirby

## Workshop in computational chemistry

## Filip Pratnicki, University of Szczecin, Poland

Explicitly correlated wavefunctions in quantum chemistry

#### 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 submission deadline: April 15, 2019.

The abstract template will be available on the conference website.

Abstract submission deadline: May 15, 2019.

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  $MC^2$ -31 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
- conference trip and dinner
- coffee or juice at breaks
- IUC reception party

### Registration fee

Before April 15, 2019:  $180.00 \in (80.00 \in \text{for students*}) + 25\% \text{ VAT}$ .

After April 15, 2019: 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 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 Vančík

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

#### ACCOMMODATION AND TRANSPORTATION

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. Information regarding reservations of accommodation and other tourist matters can be obtained by e-mailing to:

Mrs. Danijela Štrman danijela.strman@gulliver.hr

There are special prices for private accommodation in Dubrovnik for all the IUC conferences participants. For more information contact please Mrs. Danijela Štrman in Gulliver travel company. City of Dubrovnik can be reached by air from Zagreb and most of the 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.

# Registration Form MC<sup>2</sup> 31, 2019

Conference website: http://www.pmf.unizg.hr/chem/mathchemcomp Accommodation info: http://www.iuc.hr/private-accomodation.php

http://www.iuc.hr/hotels.php danijela.strman@gulliver.hr

Please send filled form to e-mail: vancik@chem.pmf.hr

Title and Attendee's Name:
Institution and VAT number:
Address of Institution:
E-mail:
Attending Workshop:
Oral presentation
Poster presentation