



# Math/Chem/Comp 2018

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

Inter University Centre Dubrovnik

18 – 23 June 2018

### CONFERENCE PROGRAM

#### MONDAY, 18 June

08:30–9:30 Registration (IUC, Don Frane Bulića 4, Dubrovnik)

9:30–10:00 **H. Vancik** and **J. Cioslowski** *Conference opening*

10:00–10:15 --- [coffee break] ---

10:15–11:15 **T. Hrenar**, *Multi-way analysis of potential energy surfaces*

11:15–12:15 **J. Cioslowski**, *Solitonic natural orbitals*

12:15–13:15 **H. Witek**, **J. Langer**, **B.-G. He**, **G. Pestka**  
*Analytical form of helium wave function*

#### TUESDAY, 19 June

8:30–9:30 **D. Fijan**, **M. Wilson**, *Structural origin of thermodynamic anomalies in liquids*

9:30–10:30 **M. V. Putz**, **P. Svera**, **M. L. Iorga**, *Modeling the bonding of quantum dots (bondots) on fullerene-graphene by Raman spectroscopy*

--- [coffee break] ---

10:45-11:45 **J. L. Andersen, Ch. Flamm, D. Merkle, P. Stadler**, *Exploring and evaluating reaction mechanisms using graph transformation*

11:45-12:45 **B. Lučić**, *The use of square of correlation coefficient ( $q^2$ ) for estimating the quality of models in chemistry: a 30 years old question*

13:00 IUC RECEPTION

16:00 – 18:00 **S. Tomić**, *Computer Aided Design of Bio-macromolecular Systems*  
**Workshop**

WEDNESDAY, 20 June

8:30-9:30 **I. Kodrin, M. Đaković, M. Čakić-Semenčić, L. Barišić**, *Computational chemistry methods as a tool for analysis and prediction of supramolecular interactions in coordination compounds*

9:30-10:30 **M. Solá, J. Poater, C. Viñas, F. Teixidor** *Linking hydrocarbon and boron hydride chemistries and bidimensional and threedimensional aromaticities*

--- [coffee break] ---

10:45-11:45 **H.-U. Siehl**, *The Conundrum of the  $C_4H_7^+$  Cation*  
*(Dedicated to George A. Olah)*

11:45-12:45 **J. Karwowski, H. A. Witek**, *Semi-exact, quasi-exact and conditionally-exact solutions of the Schrödinger equation,*

14:00 CONFERENCE TRIP

**THURSDAY, 21 June**

9:00-10:00 J. Tošović, S. Marković, *Behavior of chlorogenic acid dianion towards free radicals in water solution*

10:00-11:00 U. Bren, M. Gladović, M. Bren, *Microwave irradiation enhances misfolding of peptides*

--- [coffee break] ---

11:30-12:30 H. Vančik, I. Biljan, P. Bibulić, K. Varga, I. Rončivić, Z. Mihalić, *Reactions in crystalline solids: activation parameters and the nature of transition state*

12:30-13:30 I. Biljan, P. Bibulić, K. Varga, I. Rončivić, H. Vančik *Aromatic dinitroso derivatives: interactions through azodioxide bonds in solution, solid state and on gold surface*

**FRIDAY, 22 June**

9:00-12:00 poster session

**SATURDAY, 23 June**

11:00 Conference summary / discussions / closing