

27th MATH/CHEM/COMP

Interuniversity Centre Dubrovnik

12 – 19 June 2015

12 June (Fri) 19:00 – 20:30 Registration (Hotel Lero)

13 June (Sat) 8:30 – 9:30 Registration (IUC)

9:30 Conference opening

9:30-10:00 Word from organizers [Vančik/Cioslowski]

10:00-10:30 REMINISCENCES ON ANTE GRAOVAC - SPIRITUS MOVENS OF MCC

Dražen Vikić-Topić

10:30 [coffee break]

CHAIRMAN: J. M. Ugalde

11:00-12:00 Jens Petersen, *Simulation and control of light-induced dynamics in complex molecular systems.*

12:00-13:00 Paul G. Mezey, *How to play a piano like a violin? Integer parameters as continuous variables in molecules, anti-quantization, re-quantization, and the universal molecule modes.*

13:00-14:00 Jerzy Cioslowski, *One-electron reduced density matrices of strongly correlated harmonium atoms.*

14 June (Sun)

CHAIRMAN: J. Petersen

9:00-10:00 Hrvoj Vančik, *Chemical bonds and topochemical effects.*

10:00-11:00 Dražen Vikić-Topić, *Studies on deuterium isotope effects in ¹³C_{mn}r spectroscopy.*

11:00-11:30 [coffee break]

CHAIRMAN: D. Vikić-Topić

11:30-12:30 Urban Bren, *Cooperative binding of aflatoxin B₁ by cytochrome P450 3A4.*

12:30-13:30 Nenad Raos, *Reliability of the stability constants prediction by topological index ³χ^v.*

13:30-14:30 Pierre Hansen, *Edge realizability of chemical graphs.*

19:30 Conference dinner, Hotel LERO

15 June (Mon)

CHAIRMAN: J. Cioslowski

9:00-10:00 Damir Vukičević, *Mathematical research of molecular descriptors.*

10:00-11:00 Nino Bašić, *Iterated altans and their properties.*

11:00-12:00 Joanna Albin, *A charge-granularity correction to the electrostatic self-energy of a charge distribution in two dimensions.*

12:00-12:30 [coffee break]

CHAIRMAN: P. G. Mezey

12:30-13:30 Dragutin Svrtn, *Mixed atiyah determinants for graphs in the Euclidean or hyperbolic space.*

13:30-14:30 Tomica Hrenar, *Computational algorithms in conformational analysis of cyclic and non-cyclic molecules.*

16 June (Tue)

CHAIRMAN: H. Vančik

9:00-10:00 Ricardo A. Mata, *Sampling strategies for QM/MM calculations in condensed phase.*

10:00-11:00 Miquel Solà, *Molecular electriles and superelectriles.*

11:00-11:30 [coffee break]

CHAIRMAN: R. A. Mata

11:30-12:30 Jesus M. Ugalde, *Quantum molecular dynamical studies of the Li(+)-ferrocene complex.*

12:30-13:30 István László, *Self-organizing carbon structures in tight binding molecular dynamics calculations.*

16:30-19:30 COURSE Zlatko Mihalić, *Short introduction to computational chemistry.*

17 June (Wed) Conference excursion: to be scheduled

18 June (Thu)

9:00-12:00 Poster session and discussion about the future of Math/Chem/Comp

12:00 IUC Reception

19 June (Fri) 9:00-9:30 Conference closing