



**Nanoscience in Chemistry, Biology,  
Physics, and Mathematics**

# **BioNanoMathChem2017**

**SCIENTIFIC PROGRAM**

**Cluj, ROMANIA**

**June 28–30, 2017**

## Wednesday, June 28

09.00-09.30      **Opening ceremony**

### **SESSION 1**                      **Chairman: Ali Iranmanesh**

09.30-10.00    **Ali Reza Ashrafi** and Ali Ghalavand  
*Ordering chemical trees by Wiener polarity index*

10.00-10.30    **Subhash C. Basak**  
*Mathematical descriptors of molecules and biomolecules: Development and applications to characterization of chemical libraries, QSAR, drug design, nanotoxicology, and Zika peptide vaccine design*

10.30-11.00                      *Coffee Break*

### **SESSION 2**                      **Chairman: Lorentz Jantschi**

11.00-11.30    **Mohammad A. Iranmanesh** and Mahboubeh Saheli  
*On the harmonic index and harmonic polynomial of corcor domain of graphene*

11.30-12.00    **Zahra Khalaj**  
*Diamond and diamond-like carbon films: a brief review*

12.00-12.30    **Farzaneh Falahati-Nezhad**  
*Studying some thermodynamic properties of oligoacenes using forgotten index*

12.30-13.00    Andrés Bernal, Wilmer Leal, Eugenio Llanos, and **Guillermo Restrepo**  
*A categorical approach to chemical reactions*

13.00-14.00                      *Lunch (CHIOS Social Lounge)*

### **SESSION 3**                      **Chairman: Zahra Khalaj**

14.00-14.30    **István László**  
*Molecular dynamics simulation of carbon structures inside nano chambers*

14.30-15.00    **Seyed Mahdi Rezayat**  
*Toxicity assessment and regulation of nanohealth products in Iran: effectiveness and challenges*

15.00-15.30 **Modjtaba Ghorbani** and Mardjan Hakimi-Nezhaad  
*On Graovac-Pisanski index of polyhedral graphs*

15.30-16.00 *Coffee Break*

**SESSION 4**                      **Chairman: István László**

16.00-16.30 **Tomislav Došlić**  
*Computing degeneracies of the most important standard structures of polycyclic aromatic hydrocarbons*

16.30-17.00 **Xueliang Li**  
*Constructions of graphs and trees with partially prescribed spectrum*

17.00-17.30 Florina Scurtu, Cristina Bischin, Cristina Gruian, Anca Farcaş, Vlad Toma, and **Radu Silaghi-Dumitrescu**  
*Hemoglobin versus hemerythrin - based blood substitutes*

17.30-18.00 **Mircea V. Diudea**  
*Propellanes – a new class of structures*

18.00-18.30 **POSTER SESSION 1 (P1-P8)**

20.00-21.00 *Dinner (Panoramic)*

## Thursday, June 29

### SESSION 5 Chairman: Raluca Pop

- 09.00-09.30 **Lorentz Jäntschi**  
*Geometry optimization of  $NC_{24}$  cyclic polyyne cluster*
- 09.30-10.00 **Sorana D. Bolboacă**  
*Additive, multiplicative, and additive-multiplicative structure-property models. Which perform better?*
- 10.00-10.30 **Maryam Jalali-Rad** and Modjtaba Ghorbani  
*On the eigenvalues of fullerenes*

10.30-11.00 *Coffee Break*

### SESSION 6 Chairman: Modjtaba Ghorbani

- 11.00-11.30 **Ali Iranmanesh** and Nafiseh Jafarzadeh  
*A graph theoretical for analyzing DNA sequences based on codons*
- 11.30-11.50 **Csaba L. Nagy**  
*The Nano Studio software*
- 11.50-12.10 **Claudiu N. Lungu**, Melinda E. Füstös, Anamaria Orza, Gabriel Katona, Mircea V. Diudea, and Ireneusz P. Grudzinski  
*Water solvation clusters in assessing polymers toxicity*
- 12.10-12.30 I. G. Grosu, M. I. Rednic, M. Miclăuș, I. Grosu, and **A. Bende**  
*Intermolecular interactions in pyridinium – anion –  $\beta$ -hexachlorocyclohexane molecular crystals*
- 12.30-13.00 **Fatemeh Koorepazan-Moftakhar** and Ali Reza Ashrafi  
*Symmetry of Cubic Graphs*

13.00-14.00 *Lunch (CHIOS Social Lounge)*

### SESSION 7 Chairman: Mohammad A. Iranmanesh

- 14.00-14.30 **Zahra Sheibanizadeh**, Monir Niazi, and Zahra Khalaj  
*Investigating the physical properties of  $ZnFe_2O_4$  nanocrystals synthesized by co-precipitation method*
- 14.30-15.00 **Raluca Pop**  
*Theoretical investigations regarding the properties and applications of fullerenes and their precursors*

15.00-15.30	<b>Fănică Cimpoesu</b> <i>Revisiting the methods of the atomic structure. Back to the basis</i>
15.30-16.00	Zoltan Antal and <b>Paul G. Mezey</b> <i>Topological shape analysis of surroundings-induced shape-deformations of local electron density clouds in peptides and proteins</i>

16.00-16.30            **Closing Ceremony**

16.30-17.00            *Coffee Break*

17.00-18.30            **13<sup>th</sup> Annual Meeting of The International Academy of  
Mathematical Chemistry**

18.30-19.00            **POSTER SESSION 2 (P9-P15)**

20.00-21.00            *Dinner (CHIOS Social Lounge)*

## **Friday, June 30**

10.00-20.00            **Conference Trip**  
**(Departure from Hotel Universitas at 10.00 AM)**

**Book of abstracts** can be downloaded from:

<http://www.esmc.ro>

or

<http://www.chem.ubbcluj.ro/~diudea/conference/bionanomathchem2017/>

## Posters (in alphabetic order by the author)

- P1. **Soheila Abdi**  
*Effects of electromagnetic fields on human serum paraoxonase-1 activity in vitro*
- P2. **Adrian Brânzanic**, Ulf Ryde, and Radu Silaghi-Dumitrescu  
*DFT benchmarking for the correct description of spin states in bioinorganic centers. Heme vs. siroheme models of the sulfite reductase active site*
- P3. **Davoud Dorrnian** and Elmira Solati  
*On the laser ablation capability to synthesise nanostructures*
- P4. **Farzaneh Falahati-Nezhad**  
*Predicting gap energy and ionization energy of oligorylenes family based on TIM*
- P5. **Fatemeh Moosavi**, Mohammad Ebrahim Bahrololoom, Ramin Kamjou, and Ali Mirzaei  
*Enhanced photocatalytic activity of Pb and Co doped ZnO thin films prepared by sol-gel procedure for methylene blue degradation*
- P6. **Amirabbas Mosallanezhad**, Sirius Javadvpour, Molud Farsad, and Ramin Kamjou  
*Catalytic reduction of 4-nitrophenol using new Cu(0)/aromatic core dendrimer complexes*
- P7. **Majid Monemzadeh** and Salman Abarghouei Nejad  
*Gauge symmetries in constrained systems*
- P8. **Monir Niazi**, Zahra Sheibanizadeh, and Zahra Khalaj  
*Growth of ZnFe<sub>2</sub>O<sub>4</sub> nanocrystals by co-precipitation method*
- P9. **Luana F. Radu**, Amr A. A. Attia, Alexandru Lupan, and R. Bruce King  
*Bonding of carbonyl groups to the dipentatene dititanium system relating to products obtained from CO<sub>2</sub> activation*
- P10. **Somaye Razaghi** and Shervin Sahebi  
*Calculating different topological indices of idempotent graph of Zn*
- P11. **Vladimir R. Rosenfeld** and Mircea V. Diudea  
*Some polyhedral graphs of bionanotechnology interest*
- P12. Maryam Ghiyasiyan-Arani and **Masoud Salavati-Niasari**  
*Cobalt vanadate nanostructures: Size controllable synthesis, characterization and enhanced photocatalytic activity for the degradation of organic dyes*
- P13. **Beata Szeffler** and Mircea V. Diudea  
*Nano-dendrimers in early stages of crystal networks*
- P14. **Marina A. Tudoran** and Mihai V. Putz  
*Reactivity and aromaticity of polycyclic aromatic hydrocarbons' isomers*
- P15. **Elnaz Vaghri** and Davoud Dorrnian  
*Formation of few-layer graphene by pulsed laser ablation with second harmonic of ND:YAG laser in liquid nitrogen medium*