



Research WORKSHOP  
**NANO-MODELING OF STRATEGIC  
MATERIALS FOR KNOWLEDGE ECONOMY  
(NANO-MOD)**

**Edition I**  
**16-17 May 2018**  
**INVITATION-First Circular**

**Workshop Chair:** Prof. Dr. PI-1 **Mihai V. PUTZ**, PhD Dr.-Habil.

*You are kindly invited to join the NANO-MOD 2018 scientific and open forum in nano-modeling of strategic materials for Knowledge (Frontier) Economy. Its objectives are in presenting the top-to date and the promotion on fundamental research and their societal implication from the MULTIDISCIPLINAR NANO-CHEMISTRY and TECHNOLOGY level (non-limitative including the disciplines of physical-chemistry, chemical informatics, mathematical-chemistry, physical organic chemistry, nano-inorganic chemistry, biology-chemistry, biochemistry, bio-informatics, pharmaceutical chemistry, medical chemistry, ecotoxicology, geochemistry, QSAR, etc.) – along they featured applications and products distributed, marketed and driving the Business Chemistry and related post-modern industries (i.e. Nanotechnology: Engineered Atoms, Super-Materials; Biotechnology: Technologically Created and Enhanced Life-Forms and Systems; and 3D Printing: Digitally Designed, Chemically Manufactured Objects).*

Look to see you soon at West University of Timisoara NANO-MOD 2018!

## Organization

### Location:

- West University of Timisoara, Pestalozzi Str. No. 16 B
- The P02 (ground) Hall & Lounge of FEAA (Faculty of Economy & Business Administration)

### Partners:

- Faculty of Chemistry, Biology, Geography
- Biology-Chemistry (BC) Department
- Doctoral School of Chemistry
- Faculty of Economy and Business Administration
- Lab. of Structural and Comput. Phys. Chem. NanoSci QSAR
- Labs. of Environmental Advanced Researches
- Lab. Renewable Energy-Photovoltaics (INCEMC-Timisoara)
- European Society of Mathematical Chemistry (ESMC)
- International Academy of Mathematical Chemistry (IAMC)

### Workshop Committee:

Mihai V. PUTZ	Chair of the Workshop
Corina DUDA-SEIMAN	Executive Organizer
Vasile OSTAFE	BC Dept. Director
Mircea SELEGEAN	Guest Matters
Mircea DIUDEA	ESMC & IAMC President
Ottorino ORI	Scientific Secretary
Marius MIRICA	INCEMC-Timisoara

### Workshop Registration:

- NO Registration FEE!
- 1 page of Abstract with a Graphical Abstract (it will be used for the Official Poster of the Workshop Edition)
- Abstract style to confirmed participants (April 2018)

### Workshop Publication:

- Special Issue of *New Frontiers of Chemistry* (<http://www.newfrontchem.iqstorm.ro/>)

### Workshop Memento:

- Remember Prof. Dr. Adrian CHIRIAC

## TOPICS (not limitative, definite in 2<sup>nd</sup> circular)

### THE „NANOSCOPIC” APPROACH OF THE MATTER AND THE CHEMICAL BONDING. CHEMISTRY BUSINESS

#### Research topics No. 1:

-Characterization of the phase transitions in extended nano-systems (e.g. of graphenic and fullerenic types) with topological defects (e.g. by Stone-Wales rotations)

-Spectral techniques and nano-characterization of chemical bond and bonding

*-Clustering of Chemical Deliverable and Renewable, towards a longer and better life in nano-era of technovation*

### QUANTUM MODELING OF CHEMICAL STRUCTURE AND REACTIVITY. GLOCAL CHEMISTRY

#### Research topics No. 2:

- Electronegativity: the modern concept in Density Functional Theory; Chemical hardness: champion of electronegativity; quantum observability problem; quantification of maximum hardness principle in relation with the hard and soft acids and bases principle;

*-NANO-Chemistry Business goes GLOCAL: between local resources and global impact*

### TOPO-ALGEBRA OF THE CHEMICAL – BIOLOGICAL INTERACTION AND ECO- TOXICITY

#### Research topics No. 3:

-The quantitative structure-activity relationships (QSAR), SMILES modeling (Simplified Molecular-Input Line-Entry System) of the ligand-receptor interaction;

-Topologic indices and molecular graphs: new indices and their “real-life” correlations.

*-Bioeconomy: Industry for Enhanced Life-Forms and Systems*

## Program

### Workshop Speakers:

- In 2<sup>nd</sup> circular (April 2018)

### Workshop 1<sup>st</sup> day (16 May 2018):

- 10-10.30 AM: Opening & Remembering Prof. Dr. A. Chiriac
- 10.30 AM – 12AM: Works on TOPIC 1
- 12AM-13PM: Break for Brunch
- 13PM-15PM: Works on TOPIC 2
- 15PM-18PM: Timisoara city/nearby visits
- 18PM-21PM: Conference Dinner

### Workshop 2<sup>nd</sup> day (17 May 2018):

- 10-11.30 AM: Works on TOPIC 3
- 11.30 AM – 12AM: Break for Brunch
- 12AM-14PM: Posters' Session; Closing