



# BOOK OF ABSTRACTS

## COST Training School

COST action CA21101 COSY

**Multiscale modeling of the properties  
of compounds: From isolated  
molecules to 3D materials relevant for  
industrial and astrophysical  
applications**



Belgrade, 19<sup>th</sup> – 22<sup>nd</sup> September, 2023

The Training School of COST action CA21101 COSY

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# **BOOK OF ABSTRACTS**

Design, layout, copy-editing, and typesetting (*August-September 2023*)  
by Ivana S. Đorđević & Dragan M. Popović

# **Welcome Message**

*We are pleased to welcome you all to the first Training School of the COST Action CA21101 - CONFINED MOLECULAR SYSTEMS: FROM A NEW GENERATION OF MATERIALS TO THE STARS (COSY).*

*The Training School "Multiscale modeling of the properties of compounds: From isolated molecules to 3D materials relevant for industrial and astrophysical applications" will cover the expertise in a broad field of multiscale modeling. The topics will include physical and chemical aspects of multiscale modeling of solids, gases, liquid mixtures, fluid-structure interaction and biopolymers (proteins and nucleic acids), focusing on a better understanding and recognition of issues relevant to the application of the novel computational approaches for modeling molecular systems either isolated or in confined environments, which may consist of enclosing molecular cages, surfaces, interfaces as well as of strong electromagnetic static or optical fields. Accurate characterization of phenomena of astrochemical relevance, using the most advanced spectroscopic techniques and the highest-level ab initio theories will also be included. The Training School will address modern problems where the system complexity involves multiple time scales. As a result, the scientific program is very broad. To achieve aims of the Training School we have a great team of eminent teachers from Spain, France, Switzerland, Italy, Sweden, Romania, Czech Republic and Serbia.*

*The scientific program consists of four days of lectures, complemented by exercises aimed to provide a practical insight into the selected problems from the different covered fields. We have also scheduled a poster session, where the trainees will have the opportunity to present their work, promote themselves and create new synergies with other attendees. We are grateful to the sponsors, colleagues and friends for helping with the organization of this Training School. In particular, we are thankful to the COST Action CA21101 "COSY" for having provided the financial support, and especially to the COST Action Chair (Prof Maria Pilar de Lara-Castells) and Grant Holder (Prof Juan Carlos Hernandez-Garrido); the host institution (Institute for Chemistry, Technology and Metallurgy) in Belgrade, Serbia, for all the human, logistic, and complementary funding resources provided.*

*We would also like to express our gratitude to all of our teachers and all trainees for coming to this meeting and hope that you will have a very pleasant stay in Belgrade and plenty of interesting scientific discussions.*

*The Chairs of the 1<sup>st</sup> COSY Training School:*

*Sonja Grubišić and Jiří Vaniček*

### ***Scientific Organizing Committee:***

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| Sonja Grubišić | University of Belgrade, Institute of Chemistry, Technology and Metallurgy             |
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| Dragan Popović | University of Belgrade, Institute of Chemistry, Technology and Metallurgy             |
| Anita Lazić    | University of Belgrade, Innovation Centre of the Faculty of Technology and Metallurgy |

### ***Supported by:***



## Synthesis and characterization of Mn(II) and Fe(III) complexes with the condensation product of thiosemicarbazide and 2-acetylthiazole

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The HL ligand, (E)-2-(1-(thiazol-2-yl)ethylidene)hydrazine-1-carbothioamide, was obtained from the condensation reaction of thiosemicarbazide and 2-acetylthiazole in water. The reaction of the HL ligand with the metal salt  $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$  in a molar ratio 1:1 in methanol/water mixture results in the formation of bis Mn(II) complex with composition  $[\text{MnL}_2]$ . Complex 1 crystallizes in the triclinic crystal system with space group  $P\bar{1}$ . The Mn(II) ion is hexacoordinated with two tridentate ligands L through NNS sets of donor atoms. The geometry around the Mn is described as a distorted trigonal prism (Fig. 1).

The reaction of the ligand HL with  $\text{Fe}(\text{BF}_4)_2 \cdot 6\text{H}_2\text{O}$  in a molar ratio 1:1 in methanol results in the formation of bis Fe(III) complex with composition  $[\text{Fe}(\text{L})_2]\text{BF}_4 \cdot \text{H}_2\text{O}$ . The Fe(III) ion with L form six-coordinate complex in which two deprotonated ligand molecules coordinate in a mer arrangement, forming a distorted octahedral complex by chelation through NNS sets of donor atoms (Fig. 1). Complex 2 crystallizes in the orthorhombic crystal system with space group  $Pbca$ .



Fig 1. Molecular structure of complex 1  $[\text{MnL}_2]$  (left) and complex cation 2  $[\text{Fe}(\text{L})_2]^+$  (right).