

Jordi Cirera, Spain

„Metalloenzymes as teaching tools for coordination chemistry:

From bonding to spectroscopy“

In this presentation, we will introduce the use of metalloenzymes as illustrative examples in different fields of coordination chemistry. We will start by surveying the Protein Data Bank (PDB), and its associated tools, to later move to selected examples in which the student can use this open database to extract information that illustrates bonding, electronic structure and spectroscopic theoretical concepts usually taught in Inorganic Chemistry courses.

Béla Gyurcsik, Hungary

**„Experiences with zinc(II) containing artificial metalloproteins
and metalloenzymes“**

Artificial nucleases (ANs) can induce DNA repair within cells by hydrolysing the phosphodiester group. We designed novel integrated zinc finger nucleases: these are constructed from the inactivated C-terminal, zinc containing catalytic centre and the N-terminal allosteric activator sequence of the colicin E7 nuclease domain, which are linked to the two opposite termini of a zinc finger (ZF) array by linker sequences to achieve the optimal protein-DNA interaction. By optimizing the interactions between the two termini of the protein we can introduce regulation at various levels.

Open Discussion Session, Spain, Hungary, Poland, Bulgaria

„Featuring New (Common) Horizons“

Presentation of research groups activities and discussion on strengthening the collaboration between Universities.

Vasil Simeonov, Bulgaria

„The Philosophy of Fake Science“

The lecture makes an attempt to present the specific position in scientific forgery in the modern society. The fake science is only one of the many cases of lack of correlation between reality and good career practices for those who elected research as a profession and dedication. Different examples are presented to illustrate the foundations of the scandalous behavior in science due to manipulation and fabrication of results, plagiarism, stealing of colleague's work, ideological dogmas, experimental errors, wrong theories etc.

TRAINING SCHOOL 3

"BIO – COMP – CHEM"



24.09-28.09.2018

Bansko, Bulgaria

project BG05M2OP001-2.009-0028

"Achievement of optimal environment for education, research, innovation and sustainable development of the human source in the field of chemical sciences:
Adaptation of the today education for tomorrow"

Program

Abstracts

24.09	15.00	Departure Sofia - Bansko	
		Dinner	
25.09	Hall PIRIN		
	9.30-10.30	Vasil Simeonov	„Historical, social and metrical aspects of sustainability“
		Coffee break	
	11.00-12.00	Jorge Echeverría	„Structural databases and electronic structure methods in the study of chemical bonding“
		Lunch	
	Hall VITOSHA		
	14.00-15.30	Sergio Madurga	„Introduction to programming in Python for chemists“
		Coffee break	
	16.00-17.30	Sergio Madurga	„Introduction to programming in Python for chemists“
	Hall PIRIN		
	14.30-15.30	Błażej Kudlak	“Introducing ecotoxicology into a curriculum of the GUT - future perspectives”
		Coffee break	
16.00-17.00	Marek Tobiszewski	“Assessments and metrics for green chemistry”	
	Dinner		
Hall PIRIN			
26.09	9.30 – 10.30	Jordi Cirera	„Metalloenzymes as teaching tools for coordination chemistry: From bonding to spectroscopy“
		Coffee break	
	11.00-12.00	Béla Gyurcsik	“Experiences with zinc(II) containing artificial metalloproteins and metalloenzymes”
		Lunch	
	14.00 – 15.30	Open Discussion Session “Featuring New (Common) Horizons”	
		Coffee break	
	16.00-17.00	Vasil Simeonov	„The Philosophy of Fake Science“
	Dinner		
27.09	9.00-19.00	Social program	
	Dinner		
28.09	11.00	Departure Bansko - Sofia	

Vasil Simeonov, Bulgaria

„Historical, social and metrical aspects of sustainability“

The lecture reveals the options for creating a specific metric for assessing the sustainability issues in all of its branches – social, economic and environmental. Some interesting historical lessons related to the problem with the sustainable development are also included in order to stress the constant important and development of the sustainability tasks in every aspect of technological progress, economic growth and environmental impacts. The role of environmentrics as a capable tool for sustainability metrics is discussed and illustrated by two case studies.

Jorge Echeverría, Spain

„Structural databases and electronic structure methods in the study of chemical bonding“

Noncovalent interactions have attracted much interest in recent years due to their key role in many chemical and biological processes. The increasing computational power and the access to structural databases with thousands of references have been fundamental tools for the development of the field. This theoretical approach is explained here in detail and several applications to specific examples are also provided.

Sergio Madurga, Spain

„Introduction to programming in Python for chemists“

A practical session will be given to start to program in Python for Linux and Windows users. Example codes related to some chemistry topics will be analyzed, modified and executed using the web based Notebook environment.

Błażej Kudlak, Poland

„Introducing ecotoxicology into a curriculum of the GUT - future perspectives”

Environmental pollution plays more and more important role in awareness of modern societies and policy makers. Since decades scientists know that not only instrumental studies but also biological methods must be taken into account if one wants to give holistic information on condition of the environment. During the lecture the basic definition related to ecotoxicity will be given together with examples of utilizing wide batteries of bioassays into both model and real samples studies. Also curriculum of GUT dealing with teaching ecotoxicity will be presented.