The 1st WG2 Virtual meeting

COST action CA21101 COSY

BOOK OF ABSTRACTS

From quantum to classical dynamics of isolated molecules and 3D materials

cost
EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

COSY
COST ACTION

6th February 2024, Belgrade

The 1st Virtual meeting WG2 of COST action CA21101 COSY

From quantum to classical dynamics of isolated molecules and 3D materials

6th February 2024, Belgrade, Serbia

BOOK OF ABSTRACTS

Design, layout, copy-editing, and typesetting (*January - February 2024*)
by Ivana S. Đorđević & Dragan M. Popović

Welcome Message

We are pleased to welcome you all to the first Virtual WG2 Meeting of the COST Action CA21101 - CONFINED MOLECULAR SYSTEMS: FROM A NEW GENERATION OF MATERIALS TO THE STARS (COSY).

This one-day virtual meeting entitled "From quantum to classical dynamics of isolated molecules and 3D materials" will be dedicated to a better understanding and recognition of issues relevant to describing intermolecular interactions and molecular motion in a confining environment. The goal is to present recent advances in quantum and classical dynamics to treat molecules either isolated or in a confined environment, which may consist of enclosing molecular cages, surfaces, and interfaces as well as of strong electromagnetic static or optical fields. Speakers will be allotted 12 minutes for presentations plus 3 minutes of discussion. Also, there will be poster presentations supported by 3' time flash presentations. Presentations by young researchers are encouraged as well as those addressing specifically COST Action Goals for the 2nd Grant Period.

We are grateful to colleagues and friends for helping with the organization of this WG2 Virtual Meeting. 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 like to express our gratitude to all speakers and participants for attending this meeting and hope that we will have a very inspiring scientific program with plenty of interesting scientific discussions.

The Chairs of the 1st COSY WG2 Virtual Meeting: *Sonja Grubišić and Jiří Vaníček*

(WG2 Leaders)

Scientific Organizing Committee:

María Pilar de Lara-Castells	Consejo Superior de Investigaciones Científicas - CSIC, Spain
Cristina Puzzarini	University of Bologna, Italy
Sonja Grubišić	University of Belgrade, Institute of Chemistry, Technology and Metallurgy - ICTM, Serbia
Jiří Vaníček	Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland
Majdi Hochlaf	Université Gustave Eiffel, COSYS/IMSE, France
Francesca Mocci	University of Cagliari, Italy
Juan Carlos Hernández Garrido	Universidad de Cádiz, Spain
Vladimir Srećković	Institute of Physics Belgrade, University of Belgrade, Serbia

Local Organizing Committee:

Sonja Grubišić	University of Belgrade, Institute of Chemistry, Technology and Metallurgy
Ivana Đorđević	University of Belgrade, Institute of Chemistry, Technology and Metallurgy
Dragan Popović	University of Belgrade, Institute of Chemistry, Technology and Metallurgy
Snežana Spasić	University of Belgrade, Institute of Chemistry, Technology and Metallurgy

Supported by:

Funded by the European Union

cost EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

COSY COST ACTION

CONTENT

TALKS

Protein environment – cofactor interactions in redox protein systems

Dragan M. Popović [1]

[1]*Department of Chemistry, University of Belgrade – Institute of Chemistry, Technology and Metallurgy – National Institute of the Republic of Serbia, Belgrade*

The interactions between the enclosed protein environment and cofactors are crucial in understanding redox protein systems. The redox potential (E_m) is a key parameter of all redox-active proteins and is easily accessible in experimental and computational studies [1–3]. Synthetic bioinspired heme proteins studied here are valuable model systems in structural/functional studies and have potential for various biomedical and bionanotechnological applications [4]. The minimalistic modeling concept of synthetic enzymes provides an ideal framework for studying physicochemical properties, catalytic functions, and complex molecular processes in a simplified format. By advanced computational methods [5–7], this research examined in-depth the complex relationship between a confined protein system and its cofactor within a bioinspired protein scaffold and found multiple contributing factors. The E_m values were dissected to identify interactions in heme proteins that contribute to various energy terms. The analysis revealed significant effects of the charged protein residues, polar groups, backbone charges and orientation, inhomogeneous dielectric environments, screening effects of bulky hydrophobic sidechains, and specific mutations on heme redox properties. However, these impacts showed different weights, magnitudes, and importance [4]. This study showcases the potential of utilizing a synergistic computational and modeling methodology to develop customized proteins with predetermined functionalities and redox properties. The underlined approach could offer significant opportunities in protein engineering and design and provide fresh and exciting perspectives on this captivating field of study.

Acknowledgements:

This research has been financially supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grant No. 451-03-47/2023-01/200026). The author thanks the COST Action CA22143 "European Materials Informatics Network" (EuMINe), as well as the COST Action CA21101 (COSY) of the European Community for support.

References:

1. D. M. Popović, S. D. Zarić, B. Rabenstein, E. W. Knapp, *J. Am. Chem. Soc.* (2001), **123**, 6040.
2. D. M. Popović, A. Zmirić, S. D. Zarić, E. W. Knapp, *J. Am. Chem. Soc.* (2002), **124**, 3775.
3. D. M. Popović, A. A. Stuchebrukhov, *J. Am. Chem. Soc.* (2004), **126**, 1858.
4. D. M. Popović, *Struct. and Funct. of Cytochromes* (2022), 229–274. New York: Nova Science Publishers.
5. D. M. Popović, *Struct. and Funct. of Cytochromes* (2022), 183–228. New York: Nova Science Publishers.
6. D. M. Popović, *Struct. and Funct. of Cytochromes* (2022), 127–181. New York: Nova Science Publishers.
7. D. M. Popović, *Adv. in Biology*. Volume **2** (2022), 1–66. New York: Nova Science Publishers.