The 1st WG2 Virtual meeting

COST action CA21101 COSY

BOOK OF ABSTRACTS

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

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EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

COSY
COST ACTION

6th February 2024, Belgrade

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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
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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

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COSY COST ACTION

L19	**Vasiliu Tudor**	Exploring the Impact of PEG Length on PEI Binding to DNA: Insights from an In Silico Study of PEI-PEG-Squalene-dsDNA Polyplex Formation. The importance of using the correct simulation protocol
L20	**Nađa Došlić**	What do we get by breaking the Kasha rule?
L21	**Razvan Puf**	Investigating the influence of polyamines on G-Quadruplex structures: Insights from Molecular Dynamics
L22	**Aamir Saeed**	Exploring potential HDAC's inhibitors for halting cancer progression: insight from virtual screening, molecular docking, and molecular dynamic simulation

Poster Presentations:

P1	**Narcis-Iulian Cibotariu**	Computational analysis of the impact of polyethylene glycol-associated tert-butoxycarbonyl group in the formation, stabilization and drug encapsulation efficiency of PEGylated squalene micelles
P2	**Marinella Striccoli**	Advancing colloidal synthetic routes for carbon dots: a priori design of their optical properties
P3	**Anzhela Veselinova Marinova**	Study of the Λ-doublet population in the $O(^3P) + D_2 \rightarrow OD(^2\Pi) + D$ reaction
P4	**Žyginta Einorytė**	Modelling Glibenclamide in Aqueous Mixtures of Bioactive Ionic Liquids
P5	**Vladimir Srecković**	New data for confined molecular systems and astrochemical modelling
P6	**Einaras Sipavičius**	Modelling intermolecular structure and NMR parameters of the $[C_4mim][NO_3]$ ionic liquid and of its mixtures with water
P7	**Jafar Guliyev**	Preparation of macroporous honeycomb alumina ceramics used for water purification
P8	**Ana Isabel Furtado**	Rational design of $ScCO_2$-assisted Bio-Molecularly Imprinted Polymers
P9	**Yeha Lee**	Two-dimensional nonadiabatic quantum dynamics of the oxidation of subnanometric Cu_5 clusters
P10	**Anita Lazić**	Quantitative Crystal Structure Analysis of A Selected Spirohydantoin Derivative
P11	**Peter A. Georgiev**	Intramolecular dynamics of micropore confined CO_2 by Raman scattering

ABSTRACTS OF POSTER PRESENTATIONS

Quantitative Crystal Structure Analysis of A Selected Spirohydantoin Derivative

Anita M. Lazić,[1] Lidija D. Radovanović,[1] Jelena R. Rogan,[2] Nataša V. Valentić,[2] Ivana S. Đorđević,[3] Nemanja P. Trišović [2]

[1]*Innovation Center, Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia,*
[2]*Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia,*
[3]*University of Belgrade - Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia, Belgrade, Serbia*

An analysis of structural features of new compounds with multiple hydrogen-bond donating and accepting groups can enhance our understanding of development of supramolecular assemblies with potential for application in life sciences. Using the quantum chemical calculations, formation of the crystal structure of cyclohexane-5-spirohydantoin bearing a 4-*tert*-butylbenzoyl group (Fig. 1) was analysed in terms of a number of dimeric motifs associated with intermolecular interactions. The crystal structure retains the motif commonly found in hydantoin derivatives, where two molecules related by inversion are linked by a pair of N–H···O hydrogen bonds [1]. This motif is involved in two types of double chains, which further form a layer. Together with the dispersion interactions (π–π and hydrophobic), C–H···O interactions act as the source of attraction between the layers. Intermolecular interactions were also investigated using the Hirschfield surface analysis, enabling to additionally estimate quantitative contributions of intermolecular interactions to the crystal packing.

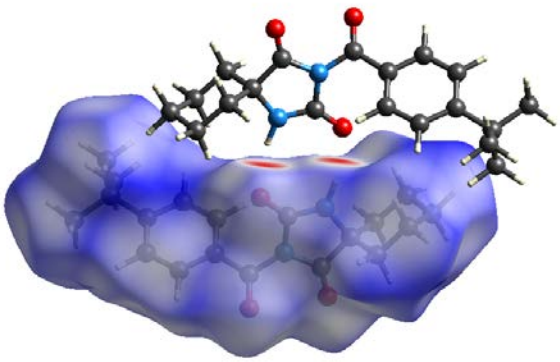

Fig 1. Structure of the investigated compound.

References:

1. A. J. Cruz-Cabeza and C. H. Schwalbe, *New J. Chem*. (2012), **36**, 1347.