

PolyChar World Forum on Advanced Materials 30th Edition



Parallel Session

From Molecules to Complex Systems with Multiscale Modelling

WEDNESDAY, September 11	11⁰⁰ – 13⁰⁰	Session B1 – ICMPP Moldova Conference Room Chair: Dr. Mariana PINTEALA
	11⁰⁰ – 11³⁰	B.PL1. MODELLING WATER IN BIOLOGY <u>Aatto LAAKSONEN</u> , ¹⁻⁴ Andrei NEAMTU, ² Tudor VASILIU, ² Dragos ISAC, ² Dragos PEPTANARIU, ² Razvan PUF, ² Petru TIRNOVAN, ² Narcis CIBOTARIU, ² Teodora RUSU, ² Mariana PINTEALA, ² Francesca MOCCI ⁴ ¹ Department of Materials and Environmental Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, Sweden ² Center of Advanced Research in Bionanoconjugates and Biopolymers, Petru Poni Institute of Macromolecular Chemistry, Romanian Academy, Iasi, Romania ³ Energy Engineering, Division of Energy Science, Luleå University of Technology, Luleå, Sweden ⁴ Department of Chemical and Geological Sciences, University of Cagliari, Monserrato (CA), Italy
	11³⁰ – 11⁴⁵	B.OC1. DFT-BASED EXPLORATION OF GRAPHENE QUANTUM DOTS IN THE ELECTROCHEMICAL OXYGEN REDUCTION REACTION <u>Isabela-Costinela MAN</u> , ¹ Raluca JALBA, ¹ Dragos-Lucian ISAC, ^{1,2} Yuheng ZHAO, ³ Ionut TRANCA ³ ¹ Costin D. Nenitescu Institute of Organic and Supramolecular Chemistry, Romanian Academy, Bucharest, Romania ² Petru Poni Institute of Macromolecular Chemistry, Romanian Academy, Iasi, Romania ³ General Chemistry - Materials Modelling Group, Vrije Universiteit Brussel, Belgium
11⁴⁵ – 12⁰⁰	B.OC2. FORMATION OF RADICAL SPECIES UNDER UV IRRADIATION IN UROCANIC ACID: AN EXPERIMENTAL AND THEORETICAL ANALYSIS OF ITS ROLE IN SKIN CANCER	

Dragos Lucian ISAC,¹ Petru TIRNOVAN,¹ Mihaela SILION,¹ Adina COROABA,¹ Teodora RUSU,¹ Mariana PINTEALA,¹ Aatto LAAKSONEN^{1,2}

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12⁰⁰ – 12¹⁵

B.OC3. INSIGHTS INTO ELECTRONIC STRUCTURE AND METAL-LIGAND BONDING IN F-ELEMENT SYSTEMS THROUGH COMPUTATIONAL X-RAY ABSORPTION SPECTROSCOPY

Dumitru-Claudiu SERGENTU,^{1,2} Ionel HUMELNICU,¹ Jochen AUTSCHBACH³

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²RECENT AIR Lab. RA-03 Alexandru Ioan Cuza University of Iasi, Iasi, Romania

³Department of Chemistry, State University of New York at Buffalo, Buffalo NY, USA

12¹⁵ – 12³⁰

B.OC4. APPLICATION OF MOLECULAR DYNAMIC SIMULATION IN SUPRA-MOLECULAR CHEMISTRY: FROM DNA-POLYCATION INTERACTIONS TO POLYMER COATED NANOPARTICLES

Tudor VASILIU,¹ Razvan PUF,¹ Francesca MOCCI,² Bogdan F. CRACIUN,¹ Sergiy PEREPELYTSYA,³

Adina COROABA,¹ Denisse BOSTIOG,¹ Mariana PINTEALA,¹ Aatto LAAKSONEN^{1,4}

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12³⁰ – 12⁴⁵

B.OC5 ENHANCING PHARMACOKINETICS OF ANTICANCER DRUG 5-FLUOROURACIL VIA LIPOSOMAL FORMULATIONS: AN INTEGRATED MULTISCALE SIMULATION AND EXPERIMENTAL STUDY

Roxana-Maria AMARANDI,¹ Luminita MARIN,^{1,2} Brindusa DRAGOI,^{1,3} Andrei NEAMTU¹

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12⁴⁵ – 13⁰⁰

B.OC6. EXPLORING COMPLEX SOLUTIONS: USING MOLECULAR DYNAMICS SIMULATIONS TO EXPLAIN UNEXPECTED CHEMICAL-PHYSICAL PROPERTIES

Francesca MOCCI¹

¹University of Cagliari, Cagliari, Italy

13⁰⁰ – 14³⁰ Lunch Break - Library Hall ICMPP

14³⁰ – 16⁰⁰

Session B2 – ICMPP Moldova Conference Room

Chair: Dr. Teodora RUSU

14³⁰ – 15⁰⁰ **B.PL2. STRUCTURING AND DYNAMICS OF METALLIC AND MOLECULAR FLEXIBLE COUNTERIONS AROUND THE DNA DOUBLE HELIX: MOLECULAR DYNAMICS INSIGHTS**

Sergiy M. PEREPELYTSYA¹

¹*Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine, Kiev, Ukraine*

15⁰⁰ – 15¹⁵ **B.OC7. MODELING AND OPTIMIZATION OF HYBRID ADSORPTION-ULTRAFILTRATION PROCESS FOR NITRITE ION REMOVAL: CHEMOMETRIC APPROACH VS. MACHINE LEARNING**

Corneliu COJOCARU¹

¹*Petru Poni Institute of Macromolecular Chemistry, Romanian Academy, Iasi, Romania*

15¹⁵ – 15³⁰ **B.OC8. DRUGCENTRAL: AN OPEN-ACCESS DATABASE OF APPROVED DRUGS SUPPORTING DRUG DISCOVERY AND REPOSITIONING**

Ramona CURPAN,¹ Sorin AVRAM,¹ Liliana HALIP,¹ Alina BORA,¹ Ana BOROTA,¹ Tudor I. OPREA²

¹*Computational Chemistry Department, Coriolan Dragulescu Institute of Chemistry, Timisoara, Romania*

²*Expert Systems Inc, San Diego, CA, USA*

15³⁰ – 15⁴⁵ **B.OC9. DRUG REPURPOSING FOR HEART FAILURE TARGETING GSK-3 β AND SGLT2 USING COMPUTATIONAL METHODS**

Alexandru SAVA¹, Bianca-Stefania PROFIRE², Geanina Florentina LUPASCU¹, Lenuta PROFIRE¹

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²*Faculty of Medicine, GT Popa University of Medicine and Pharmacy of Iasi, Iasi, Romania*

15⁴⁵ – 16⁰⁰ **B.OC10. IN SILICO STUDIES OF NEW HETEROCYCLIC DERIVATIVES TARGETING NEURODEGENERATIVE DISEASES**

Iulian CALUIAN¹, Andreea Teodora IACOB¹, Lenuta PROFIRE¹

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