

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	<p>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 MOCCI⁴ ¹<i>Department of Materials and Environmental Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, Sweden</i> ²<i>Center of Advanced Research in Bionanoconjugates and Biopolymers, Petru Poni Institute of Macromolecular Chemistry, Romanian Academy, Iasi, Romania</i> ³<i>Energy Engineering, Division of Energy Science, Luleå University of Technology, Luleå, Sweden</i> ⁴<i>Department of Chemical and Geological Sciences, University of Cagliari, Monserrato (CA), Italy</i></p>
11³⁰ – 11⁴⁵	<p>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 TRANCA³ ¹<i>Costin D. Nenitescu Institute of Organic and Supramolecular Chemistry, Romanian Academy, Bucharest, Romania</i> ²<i>Petru Poni Institute of Macromolecular Chemistry, Romanian Academy, Iasi, Romania</i> ³<i>General Chemistry - Materials Modelling Group, Vrije Universiteit Brussel, Belgium</i></p>	
11⁴⁵ – 12⁰⁰	<p>B.OC2. FORMATION OF RADICAL SPECIES UNDER UV IRRADIATION IN UROCANIC ACID: AN EXPERIMENTAL AND THEORETICAL ANALYSIS OF ITS ROLE IN SKIN CANCER</p>	

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

¹Centre of Advanced Research in Bionanoconjugates and Biopolymers, Petru Poni
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²Division of Physical Chemistry, Department of Materials and Environmental
Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, Sweden

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

¹Faculty of Chemistry, Alexandru Ioan Cuza University of Iasi, Iasi, Romania

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
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Italy

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Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, Sweden

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

¹TRANSCEND Research Center, IRO Iasi, Iasi, Romania

²Petru Poni Institute of Macromolecular Chemistry, Romanian Academy,
Iasi, Romania

³Faculty of Chemistry, Alexandru Ioan Cuza University of Iasi, Iasi, Romania

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. PERPELYTSYA¹

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 CURPAN¹, Sorin AVRAM¹, Liliana HALIP¹, Alina BORA¹, Ana BOROTA¹, 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-3B AND SGLT2 USING COMPUTATIONAL METHODS**

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

¹*Faculty of Pharmacy, GT Popa, University of Medicine and Pharmacy of Iasi, Iasi, Romania*

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

¹*Faculty of Pharmacy, G T Popa University of Medicine and Pharmacy of Iasi, Iasi, Romania*

Join Zoom Meeting

<https://us06web.zoom.us/j/79916317094?pwd=JOhzZbkiSNysK26xiHY9PBCWnlRxEU.1>

Topic: BioMat4CAST Session

Time: Sep 11, 2024 10:30 AM Bucharest

PolyChar World Forum on Advanced Materials

Iasi • Romania • September 11 - 13, 2024

**POLY
CHAR'30**

PolyChar World Forum on Advanced Materials 30th Edition

Program

<https://icmpp.ro/polychar'30/program.php>

Petru Poni Institute of Macromolecular Chemistry

Wednesday, 11.09.2024

Thursday, 12.09.2024

Friday, 13.09.2024

ICMPP Conference Hall	
S1	09:00 - 09:15 Opening
	09:15 - 09:45 Valeria HARABAGIU
	09:45 - 10:30 PL1. Kirk SCHANZE
10:30 - 11:00 Coffee break	
S2	11:00 - 11:40 L1. Witold BROSTOW
	11:40 - 12:20 L2. Cosimo CARFAGNA
	12:20 - 13:00 L3. Carmen TEODOSIU
13:00 - 14:30 Lunch break	
S3	14:30 - 15:10 L4. Jean-Francois GERARD
	15:10 - 15:50 L5. Calin DELEANU
	15:50 - 16:20 Coffee break
S4	16:20 - 17:00 L6. Kevin P. MENARD
	17:00 - 17:40 L7. Cyrille SOLLOGOUB

ICMPP Library	
BioMat4CAST Session	
B1	11:00 - 11:30 B.PL1. Aatto LAAKSONEN
	11:30 - 11:45 B.OC1. Isabela-Costinela MAN
	11:45 - 12:00 B.OC2. Petru TIRNOVAN
	12:00 - 12:15 B.OC3. Dumitru-Claudiu SERGENTU
	12:15 - 12:30 B.OC4. Tudor VASILIU
	12:30 - 12:45 B.OC5. Roxana-Maria AMARANDI
12:45 - 13:00 B.OC6. Francesca MOCCI	
13:00 - 14:30 Lunch break	
B2	14:30 - 15:00 B.PL2. Sergiy M. PEREPELYTSA
	15:00 - 15:15 B.OC7. Cornel COJOCARU
	15:15 - 15:30 B.OC8. Ramona CURPAN
	15:30 - 15:45 B.OC9. Alexandru SAVA
	15:45 - 16:00 B.OC10. Iulian CALUIAN

ICMPP Conference Hall	
S5	9:00 - 9:45 PL2. Jean-Francois GERARD
	9:45 - 10:30 PL3. Maria Cristina COCCA
10:30 - 11:00 Coffee break & Poster session	
S6	11:00 - 11:45 PL4. Conchi ANIA
	11:45 - 12:15 C1. Witold BROSTOW
	12:15 - 12:30 OC1. Veronica AMBROGI
12:30 - 14:00 Group photo Lunch break	
S7	14:00 - 14:45 PL5. Salvatore IANNACE
	14:45 - 15:15 C2. Mihai BREBU
	15:15 - 15:30 OC2. Mariana CRISTEA
15:30 - 16:00 Coffee break & Poster session	
S8	16:00 - 16:15 OC3. Riccardo MANFREDI
	16:15 - 16:30 OC4. Madalin DAMOC
	16:30 - 16:45 OC5. Cosimo BRONDI
	16:45 - 17:00 OC6. Paul-Valentin LOVIN
	17:00 - 17:15 OC7. Dragos-Lucian ISAC
	17:15 - 17:30 OC8. Pawel GNIDA
19:00 - 22:00 Dinner Traian Hotel	

ICMPP Conference Hall	
S9	9:00 - 9:45 PL6. Stergios PISPAS
	9:45 - 10:15 C3. Mihaela POP
	10:15 - 10:30 OC9. Pierfrancesco CERRUTI
10:30 - 11:00 Coffee break & Poster session	
S10	11:00 - 11:45 PL7. Rosica MINCHEVA
	11:45 - 12:15 C4. Alexandru ASANDEI
	12:15 - 12:30 OC10. Florin BUCATARIU
12:30 - 14:00 Lunch break	
S11	14:00 - 14:45 PL8. Anatoli SERGHEI
	14:45 - 15:15 C5. Aurica FARCAS
	15:15 - 15:30 OC11. Teodoro LAINO
15:30 - 16:00 Coffee break & Poster session	
S12	16:00 - 16:15 OC12. Elena STOLERU
	16:15 - 16:30 OC13. Cristina AL-MATARNEH
	16:30 - 16:45 OC14. Oana-Maria MEMECICA
	16:45 - 17:00 OC15. Angela MAROTTA
	17:00 - 17:15 OC16. Vlad TARPA
	17:15 - 17:30 OC17. Alin-Ionut ALECU
17:30 - 18:00 Awards and closing	

Legend:	PLx. Plenary Lecture	Lx. Lecture	Cx. Conference	OCx. Oral Communication
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