

BIMac 2019

COMPUTATIONAL AND EXPERIMENTAL APPROACH TO POLYMERS IN BIOLOGICAL AND SOFT MATTER

XXIII. BRATISLAVA INTERNATIONAL CONFERENCE ON MACROMOLECULES



Monday, 1st July

8:40 – 09:00 Conference Opening

Chairperson Dušan Račko

09:00 – 10:00 IL-1 M. Natália D. S. Cordeiro (Portugal)

Unravelling the Synthesis of Janus Thiol-Coated Nanoparticles by Molecular Simulations

10:00 – 10:30 CL-1 Gyorgy Hantal (Austria)

On molecular mechanisms of general anesthesia

10:30 – 11:00 Coffee Break

11:00 – 11:30 CL-2 Zuzana Benková (Slovakia)

Interactions of poly(ethylene oxide) coated carbon nanotubes with peptides

11:30 – 12:00 CL-3 Marco Krummenacher (Germany)

Interaction of amphiphilic bottle brush and star polymers with a biological membrane: A coarse-grained molecular dynamics study

12:00 – 14:00 Lunch

Chairperson M. Natália D. S. Cordeiro

14:00 – 14:30 CL-4 Giuliana Giunta (United Kingdom)

A novel Coarse-Grained Model for Entangled Polymers on Solid Surfaces

14:30 – 15:00 CL-5 Gerardo Campos-Villalobos (United Kingdom)

Coarse-grained potential derivation for modelling self-assembly of block-copolymers in binary solvents

15:00 – 15:30 CL-6 Dušan Velič (Slovakia)

Thiophene based copolymers: correlation of electron dynamics and film structure

15:30 – 16:00 CL-7 Michal Malček (Slovakia)

On the adsorption ability of Cu-doped and Cu-decorated graphene quantum dots

16:00 – 16:30 Coffee Break

16:30 – 18:00 Poster session

LIST OF POSTERS

- P-1 Giuliana Giunta**
A novel Coarse-Grained Model for Entangled Polymers on Solid Surfaces (also lecture with the same title)
- P-2 Samuel Wierzbicki**
Simulations of the kinetics of the free radical oligomerization
- P-3 Maria Pantelidou**
Coarse-grained mean field simulations of a triblock copolymer system. The effect of flexibility on the micellization behavior
- P-4 Peter Čakánek**
Molecular dynamics simulations of carbon nanotubes covered by poly(ethylene oxide) chains and their interactions with peptides
- P-5 Maria Panoukidou**
Construction of phase diagrams of anionic surfactants using dissipative particle dynamics
- P-6 Pascal Hebbeker**
Tuning the interactions of oligopeptides with star-like polyelectrolytes by means of charge regulation
- P-7 Mariarita Paciolla**
Collapse of macromolecular architectures in bad solvent: a computational study of the coarsening kinetics of microgels, stars and semiflexible chains
- P-8 Barbora Stratilová**
Stability of reaction complex of specific and nonspecific xyloglucan endotransglycosylase (XET) with linear oligosaccharides as acceptors
- P-9 Martin Blaško**
DFT modeling of cross-linked polyethylene: role of gold atoms and dispersion interactions
- P-10 Helena Švajdlenková**
Microscopic probing of amorphous polymers by means of ESR and PALS techniques: *cis*-1,4-poly(isoprene)
- P-11 Zuzana Benková**
Conformational behavior of end-grafted PEO chains as potential protection layer against protein adsorption
- P-12 Zuzana Benková**
Wetting behavior of PEO-grafted silica surface in presence of free homopolymers
- P-13 Dušan Račko**
Comparison of methods for modeling chromatin loop extrusion: constant force and constant speed motors
- P-14 Dušan Račko**
The free volume in a polymer water mixture: pol (vinyl methether) case
- P-15 Dušan Račko**
Chromatin loop extrusion and chromatin unknotting
- P-16 Kamil Tokár**
Optical and vibrational spectra of lignin monomers from DFT simulations

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Tuesday, 2nd July

Chairperson Zuzana Benková

09:00 –10:00 IL-2 Christos Likos (Austria)

Self-organization and rheology of block copolymer star solutions

10:00 –10:30 CL-8 Emanuele Locatelli (Austria)

Conformations and dynamics of polar active polymers

10:30 – 11:00 Coffee Break

11:00 –11:30 CL-9 Maria Panoukidou (United Kingdom)

Construction of phase diagrams of anionic surfactants using dissipative particle dynamics

11:30 –12:00 CL-10 Mariarita Paciolla (Spain)

Collapse of macromolecular architectures in bad solvent: A computational study of the coarsening kinetics of microgels, stars and semiflexible chains

12:00 – 14:00 Lunch

Chairperson Christos Likos

14:00 –14:30 CL-11 Peter Cifra (Slovakia)

Force-displacement relations at compression of dsDNA

14:30 –15:00 CL-12 Pascal Hebbeker (Czech Republic)

Modeling of reactive polymers: methods, pitfalls and achievements

15:00 –15:30 CL-13 Anna Zahoranová (Slovakia)

Poly(2-oxazoline) block copolymers: from temperature driven self-assembly to triggerable drug carriers

15:30 –16:00 CL-14 Stanislav Kozmon (Slovakia)

Complex theoretical study of the O-GlcNAc transferase reaction mechanism

16:00 – 16:30 Coffee Break

16:30 – 18:00 Individual Programme or Conference Trip around Bratislava Downtown

19:30 – 21:00 Conference Dinner

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Wednesday, 3rd July

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| Chairperson | Peter Cifra |
| 09:00 –10:00 | IL-3 Ján Smrek (Austria) <i>Active topological glass in relation to chromosome conformation and dynamics</i> |
| 10:00 –10:30 | CL-15 Dušan Račko (Slovakia) <i>Introducing Supercoiling into Models of DNA and Chromosome Structure</i> |
| 11:00 –11:30 | CL-16 Helena Švajdlenková (Slovakia) <i>Free volume microstructure of photopolymers studied by positron annihilation lifetime spectroscopy</i> |
| 11:30 –12:00 | CL-17 Bartosz Greń (Poland) <i>Statistical properties of lasso-shape polymers and their implications for complex lasso proteins</i> |
| 12:00 –12:20 | CL-18 Róbert Balogh (Slovakia) <i>Thiazolo[5,4-d]thiazole based small molecules with oxadiazole spacer as an electron transport materials for organic light emitting diodes</i> |
| 12:20 – 14:00 | Closing Remarks and Lunch |