Computational Physics of Confined Systems: From Life to Material Sciences

June 24-26, 2025

Program

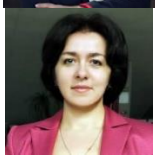
Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine **Room 322 and Zoom**

https://us06web.zoom.us/j/89631785051?pwd=g6gxmrIh4aA6Q5DJekjR2tOl4WsXTW.1

Conference ID: 896 3178 5051

Code: 616956

Tuesday, 24.06.2025

	Kyiv time	
	10-00 10-10	**OPENING** **Sergiy Perepelytsya** (Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine) **Maria Pilar de Lara-Castells** (COSY COST Action Chair) **Cristina Puzzarini** (COSY COST Action Vice Chair)
	10-10 11-10	**Aatto Laaksonen** *Stockholm University, Sweden* "Modeling polymers constrained by Nature"
	11-10 12-10	**Francesca Mocci** *University of Cagliari, Italy* "Multiscale Molecular Modeling of DNA: Toward Simulating Its Naturally Confined Environment"
	12-10 12-30	**COFFEE BREAK**
	12-30 13-30	**Sergiy Perepelytsya** *Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine* "Counterions confined in DNA nanomaterials: Insights form modeling and simulation"
	13-30 14-30	**LUNCH**
	14-30 15-30	**Sonja Grubisic** *University of Belgrade, Serbia* "Biomolecular Force Fields: Recent Advances in Nonstandard Amino Acid and Nucleic Acid Development"
	15-30 16-30	**Valeriya Trusova** *V.N. Karazin National University, Kharkiv, Ukraine* "From molecular simulations to functional design: computational insights into theranostic protein-based nanostructures"
	16-30 18-00	**Evening Scientific Mixer**

Wednesday, 25.06.2025

Kyiv time

10-00 **Anna Shestopalova**
11-00 *O.Ya. Usikov Institute of Radiophysics and Electronics of the NAS of Ukraine, Kharkiv, Ukraine*
"Drug Design and Repurposing: An Overview with Selected Examples"

11-00 **Tetiana Bubon**
12-00 *Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine, University of Trieste, Italy*
"Modeling of the Structure and Dynamics of the DNA Hydration Shell"

12-00 **COFFEE BREAK**
12-30

12-30 **Ali Hassanali**
13-30 *The Abdus Salam International Center for Theoretical Physics, Trieste, Italy*
TBA

13-30 **LUNCH**
14-30

14-30 **Dmytro Piatnytskyi**
15-30 *Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine*
"Quantum chemical calculations basics"

15-30 **Piotr Żuchowski**
16-30 *Nicolaus Copernicus University, Poland*
"Molecular interactions with quantum chemistry methods"

16-30 **Excursion for the participants attending in person**
18-00

Thursday, 26.06.2025

Kyiv time

10-00
11-00

Andrij Baumketner
Institute of Condensed Matter Physics of the NAS of Ukraine, Lviv, Ukraine
"What can we learn about quantum dots from computer simulations?"

11-00
12-00

Carlo Maria Carbonaro
Physics Department in University of Cagliari, Italy
"Experimental and computational characterization of carbon dots"

12-00
12-30

COFFEE BREAK

12-30
13-30

Valentyna Kuznetsova
Department of Physics at the University of South Bohemia in Ceske Budejovice, Czech Republic
"How to give a good presentation"

13-30
14-30

LUNCH

14-30

PARTICIPANT PRESENTATIONS

Dragan Popović
University of Belgrade – Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia
"Energetics of steps in proton pumping mechanism of cytochrome c oxidase"

Yevhen Osokin
Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine
"Features of dπ-pπ-BONDING OF Cu(I) π-complexes with some unsaturated acids"

Aamir Saeed
Department of Geological and chemical sciences, University of Cagliari
"Insights into small molecule stabilization of viral G-quadruplexes via molecular dynamics and docking simulations"

Oleksandr Perig
Donbas State Engineering Academy, Ukraine
TBA

Olha Vlasiuk, Anna Stetsyuk
National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"
"Li-DNA systems for new battery technologies"

Anita Lazić
The Innovation Centre of the Faculty of Technology and Metallurgy, University of Belgrade
"Structural effects on the antioxidant potential and drug-likeness of selected xanthene derivatives"

Giulia Olla
Department of Chemical and Geological Sciences, University of Cagliari
“Molecular dynamics simulations of 143d and 1kf1 G-quadruplexes”

Enrico Puddu
Department of Chemical and Geological Sciences, University of Cagliari
“Temperature-dependent stability of a viral G-quadruplex: a computational approach”

Zaira Carboni
Department of Physics, University of Cagliari
“Optical behavior and structural insights into nitrogen-doped carbon dots”

17-00 **Closing**