

Computational Physics of Confined Systems: From Life to Material Sciences *June 24-26, 2024*

Program

Zoom link

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

Conference ID: 896 3178 5051

Code: 616956

Tuesday, 24.06.2025

	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)
	10-10 11-10	Aatto Laaksonen Stockholm University “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 from modeling and simulation”
	13-30 14-30	Lunch
	14-30 15-30	Sonja Grubisic University of Belgrade “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



10-00
11-00

Anna Shestopalova
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
12-00

Tetiana Bubon
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
12-30

Coffee break



12-30
13-30

Ali Hassanali
The Abdus Salam International Center for Theoretical
Physics, Trieste, Italy
TBA

13-30
14-30

Lunch



14-30
15-30

Dmytro Piatnytskyi
Bogolyubov Institute for Theoretical Physics of the NAS
of Ukraine
“Quantum chemical calculations basics”



15-30
16-30

Piotr Żuchowski
Nicolaus Copernicus University, Poland
“Molecular interactions with quantum chemistry methods”

16-30
18-00

Excursion for the participants attending in person

Thursday, 26.06.2025



10-00 Andrij Baumketner
11-00 Institute of Condensed Matter Physics of the NAS of Ukraine, Lviv, Ukraine
“What can we learn about quantum dots from computer simulations?”



11-00 Carlo Maria Carbonaro
12-00 Physics Department in University of Cagliari, Italy
“Experimental and computational characterization of carbon dots”

12-00 **Coffee break**

12-30



12-30 Valentyna Kuznetsova
13-30 Department of Physics at the University of South Bohemia in Ceske Budejovice, Czech Republic
“How to give a good presentation”

13-30 **Lunch**

14-30

Participant Presentations

14-30 Dragan Popović
14-50 “Energetics of steps in proton pumping mechanism of cytochrome c oxidase”

University of Belgrade - Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia

14-50 Yevhen Osokin
15-10 “Features of $d\pi$ - π -BONDING OF Cu(I) π -complexes with some unsaturated acids”

Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine

15-10 Aamir Saeed

15-30 TBA
Department of Geological and chemical sciences, University of Cagliari

15-30 Oleksandr Perig

15-50 TBA
Donbas State Engineering Academy

15-50 Olha Vlasiuk

16-10 TBA
National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"

Closing

