

Computational Physics of Confined Systems: From Life to Material Sciences

June 25-27, 2026

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

<https://us06web.zoom.us/j/89631785051?pwd=g6gxmrIh4aA6Q5DJekjR2tO14WsXTW.1>

Conference ID: 896 3178 5051

Code: 616956

Late registration ([website](#))

Interested participants are welcome to register using the QR code below



Program

Thursday, 25.06.2026

Kyiv time

	10:00	OPENING
	10:15	Maria Pilar de Lara-Castells COSY COST Action Chair
	10:15	Sergiy Perepelytsya <i>Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine, Ukraine</i>
	11:15	Sergiy Perepelytsya <i>Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine, Ukraine</i>
	<i>In person</i>	“Molecular dynamics: from the hard-sphere problem to biomolecules”
	11:15	Ari Paavo Seitsonen <i>Ecole Normale Supérieure de Paris, France</i>
	12:15	“Computing spectroscopic responses from molecular dynamics: example case of liquid water”
	<i>In person</i>	
12:15-12:40		COFFEE BREAK



12:40

Khrystyna Gnatenko

13:40

Ivan Franko National University of Lviv, Ukraine

“Fundamentals of quantum programming and quantum computing studies of quantum and classical systems”

In person

13:40

LUNCH

14:30



14:30

Erik Laurini

15:30

University of Trieste, Italy

“Molecular dynamics for life sciences: principles, force fields, and biomolecular applications”

Online

15:30

Domenico Marson

16:30

University of Trieste, Italy

“Advanced molecular dynamics for life and material sciences: improved force fields, materials properties, and enhanced sampling”

Online



16:30

Marina Kosevich

17:00

B. Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine, Ukraine

“Interplay between mass spectrometry and computations in characterization of biomolecules”

Online



17:00

Excursion

18:00

Friday, 26.06.2026

Kyiv time



10:00

Kestutis Aidas

11:00

Vilnius University, Lithuania

“Structural and NMR properties of ionic liquid materials: insights from MD/QM modelling”

Online

11:00

Tetiana Bubon

12:00

Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine

“Water, ions, and DNA: when hydration matters”

In person



12:00-12:30

COFFEE BREAK



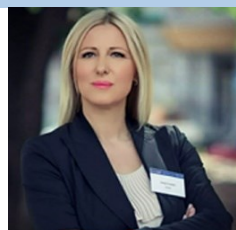
12:30
13:30

Taras Bryk
Yukhnovskii Institute for Condensed Matter Physics of NAS of Ukraine, Ukraine

Online “Collective dynamics of liquids in bulk and narrow channels”

13:30 **LUNCH**

14:30



14:30 **Sonja Grubišić**
University of Belgrade, Serbia

15:30 “Predicting gas adsorption in metal–organic frameworks using grand canonical Monte Carlo simulations”

Online

15:30 **COFFEE BREAK**

16:00



16:00 **Petra Čechová**
Czech Advanced Technology Research Institute (CATRIN), Czech Republic

17:00 “The geometry-phase relationship of lipid assemblies”

Online

Saturday, 27.06.2026

Kyiv time



10:00
11:00

Vitalii Tymshyshyn
Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine, Ukraine

In person “From neural network fundamentals to gridless computation (Part I)”

11:00 Vitalii Tymshyshyn

12:00 *Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine, Ukraine*
“From neural network fundamentals to gridless computation (Part II)”

12:00 **COFFEE BREAK**

12:30



12:30 **Francesca Mocci**
University of Cagliari, Italy

13:30 “Modeling DNA beyond the atomistic scale: coarse-grained approaches and applications”

Online

13:30 **LUNCH**

14:30

Participants' Session

14:30	Yevhen Osokin
14:50	<i>Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Ukraine</i>
	TBA
14:50	Dragan Popović
15:10	<i>University of Belgrade, Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia</i>
	“Photoactivation of DNA photolyase: intraprotein electron and radical transfer”
15:50	COFFEE BREAK
16:10	
16:10	Bogdana Reshotka
16:30	<i>Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Ukraine</i>
	TBA
16:30	Michele Fulghesu
16:50	<i>University of Cagliari, Italy</i>
	TBA
17:00	Closing