



**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

Program

Thursday, 25.06.2026

Kyiv time

10:00	OPENING
10:15	Maria Pilar de Lara-Castells COSY COST Action Chair
	Sergiy Perepelytsya <i>Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine, Ukraine</i>
10:15	Sergiy Perepelytsya
11:15	<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
12:15	<i>Ecole Normale Supérieure de Paris, France</i>
<i>In person</i>	“Computing spectroscopic responses from molecular dynamics: example case of liquid water”
12:15-12:40	COFFEE BREAK
12:40	Khrystyna Gnatenko
13:40	<i>Ivan Franko National University of Lviv, Ukraine</i>
<i>In person</i>	“Fundamentals of quantum programming and quantum computing studies of quantum and classical systems”
13:40	LUNCH
14:30	
14:30	Erik Laurini
15:30	<i>University of Trieste, Italy</i>
<i>Online</i>	“Molecular dynamics for life sciences: principles, force fields, and biomolecular applications”
15:30	Domenico Marson
16:30	<i>University of Trieste, Italy</i>

<i>Online</i>	“Advanced molecular dynamics for life and material sciences: improved force fields, materials properties, and enhanced sampling”
16:30	Marina Kosevich
17:00	<i>B. Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine, Ukraine</i>
<i>Online</i>	“Interplay between mass spectrometry and computations in characterization of biomolecules”
17:00	Excursion
18:00	

Friday, 26.06.2026

Kyiv time

10:00	Kestutis Aidas
11:00	<i>Vilnius University, Lithuania</i>
<i>Online</i>	“Structural and NMR properties of ionic liquid materials: insights from MD/QM modelling”
11:00	Tetiana Bubon
12:00	<i>Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine</i>
<i>In person</i>	“Water, ions, and DNA: when hydration matters”
12:00-12:30	COFFEE BREAK
12:30	Taras Bryk
13:30	<i>Yukhnovskii Institute for Condensed Matter Physics of NAS of Ukraine, Ukraine</i>
<i>Online</i>	“Collective dynamics of liquids in bulk and narrow channels”
13:30	LUNCH
14:30	
14:30	Sonja Grubišić
15:30	<i>University of Belgrade, Serbia</i>
<i>Online</i>	“Predicting gas adsorption in metal–organic frameworks using grand canonical Monte Carlo simulations”
15:30	COFFEE BREAK
16:00	
16:00	Petra Čechová
17:00	<i>Czech Advanced Technology Research Institute (CATRIN), Czech Republic</i>
<i>Online</i>	“The geometry-phase relationship of lipid assemblies”

Saturday, 27.06.2026

Kyiv time

10:00	Vitalii Tymshyshyn
11:00	<i>Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine, Ukraine</i>
<i>In person</i>	“From neural network fundamentals to gridless computation (Part I)”
11:00	Vitalii Tymshyshyn
12:00	<i>Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine, Ukraine</i>
	“From neural network fundamentals to gridless computation (Part II)”
12:00	COFFEE BREAK
12:30	
12:30	Francesca Mocci
13:30	<i>University of Cagliari, Italy</i>
<i>Online</i>	“Modeling DNA beyond the atomistic scale: coarse-grained approaches and applications”
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