APS Satellite Symposium & Workshop

"Applied Problems of Theoretical and Computational Biophysics"

March 17-19, 2026

Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine

PROGRAM

March 17
(Room 322 and online)

13.30 **Opening APS Satellite Symposium**

13.30 **Sergiy Perepelytsya**
«Counterions in DNA-nanomaterials» *(Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine)*

13.42 **Francesca Mocci**
«Molecular dynamics insights into the stabilization of nucleic acid quadruplexes» *(University of Cagliari, Cagliari, Italy)*

13.54 **Anna Shestopalova**
«Drug repurposing: molecular modelling» *(O. Ya. Usikov Institute for Radiophysics and Electronics, NASU, Kharkiv, Ukraine)*

14.06 **Taras Patsahan**
«Computer simulation of cell sorting on dynamic microstructured surfaces» *(Yukhnovskii Institute for Condensed Matter Physics, Lviv, Ukraine)*

14.18 **Andrij Baumketner**
«Modeling aggregation of proteins on computers» *(Yukhnovskii Institute for Condensed Matter Physics, Lviv, Ukraine)*

14.30 **Aleksei Aksimentiev**
«DNA electromotors» *(University of Illinois at Urbana-Champaign, Urbana-Champaign, USA)*

14.42 **Larissa Brizhik**
«Soliton mediated long-range electron transport in Donor–Biopolymer–Acceptor systems» *(Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine)*

14.54 **Galyna Dovbeshko**
«Spectroscopic markers of biological molecules and cells» *(Institute of Physics, NASU, Kyiv, Ukraine)*

15.06 **Victor Karachevtsev**
«Photoluminescent MoS2 quantum dots surrounded by nucleotides» *(B.Verkin Institute for Low Temperature Physics and Engineering, NASU, Kharkiv, Ukraine)*

15.18 **Khrystyna Gnatenko**
«Quantum programming for the study of complex systems, and possible applications in biophysics»
(Ivan Franko National University of Lviv)

15.30 **Eugene Kryachko**
«On measuring localization and delocalization patterns in molecules» *(Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine)*

Conference dinner

March 18
(Room 322 and online)

10.00	**Taras Patsahan** «Simulation study of affinity-based cell sorting on switchable microstructured surfaces» *(Yukhnovskii Institute for Condensed Matter Physics, Lviv, Ukraine)*
10.30	**Andrij Baumketner** «Modeling aggregation of proteins on computers» *(Yukhnovskii Institute for Condensed Matter Physics, Lviv, Ukraine)*
11.00	**Sergiy Perepelytsya** «Counterions in DNA-nanomaterials» *(Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine)*
11.30	**Coffee break**
12.00	**Marina V. Kosevich** «How could a molybdenum metal atom get into biomolecules' structure: mass spectrometry based version» *(B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine)*
12.30	**Larissa Brizhik** «Nonlinear mechanism of magnetic field impact on charge transport in macromolecules» *(Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine)*
13.00	**Khrystyna Gnatenko** «Quantum programming for the study of complex systems, and possible applications in biophysics» *(Ivan Franko National University of Lviv)*
13.30	**Lunch**
14.30	**Vlada A. Pashynska** «Bionanomaterials for drug delivery: computational and experimental study of MoS2-based nanocomposites with anticancer drugs» *(B. Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine)*
15.00	**Yaroslav Ilnytskyi** «Adsorption of the low density lipoptoteins on photo-sensitive polymer brushes: computer simulations» *(Yukhnovskii Institute for Condensed Matter Physics, Lviv, Ukraine)*

15.30 **Viktoria Blavatska**
«The effect of branching in modeling adsorption of impurities by polymeric adsorbents»
(Yukhnovskii Institute for Condensed Matter Physics, Lviv, Ukraine)

16-00 **Coffee break**

16-30 **Aleksei Aksimentiev**
«DNA Electromotors»
(University of Illinois at Urbana-Champaign, USA)

17-00 **Dmitriy M. Glibitskiy**
«Towards machine learning-based segmentation of zigzag patterns in BSA film micrographs» *(O. Ya. Usikov Institute for Radiophysics and Electronics of the National Academy of Sciences of Ukraine)*

17-30 **Oleksandr Shchehlov**
«Multifunctional nanodispersed X-ray phosphors in a drug delivery system in X-ray photodynamic therapy» *(Department of Nanomaterials, Chuiko Institute of Surface Chemistry of NAS of Ukraine)*

18.00 **Closing the Session**

March 19
(Room 322 and online)

10.00 **Galyna Dovbeshko**
«Physicochemical properties and neurotoxicity of hazardous carbon smoke nanoparticles with heavy metals» *(Institute of Physics of the National Academy of Sciences of Ukraine)*

10.30 **Olena Gnatyuk**
«Mechanical properties of circulating tumor cells as markers of metastatic activity» *(Institute of Physics of the National Academy of Sciences of Ukraine)*

11.00 **Olena Pavlenko**
«Quantum mechanical calculations in prediction of properties of π-conjugateded molecules» *(Taras Shevchenko National Uviversity of Kyiv)*

11.30 **Coffee break**

12.00 **Francesca Mocci**
«Molecular dynamics insights into the stabilization of nucleic acid quadruplexes» *(University of Cagliari, Cagliari, Italy)*

12.30 **Yevhen Osokin**
«Quantum-chemical modeling of mono- and biligand complexes of silver ions with some DNA nucleotide bases» *(Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine)*

13.00 **Anna Shestopalova**
«Drug repurposing: molecular modelling» *(O. Ya. Usikov Institute for Radiophysics and Electronics, NASU, Kharkiv, Ukraine)*

13.30 **Lunch**

14.30 **Vasyl Hurmach**
«Targeting TMPRSS2 with carbon nanostructures: an in silico study» *(Institute of Molecular Biology and Genetics, National Academy of Sciences of Ukraine)*

15.00 **Taras Voitsitskyi**
«Protein-ligand docking with machine learning» *(Institute of Physics of the National Academy of Sciences of Ukraine)*

15.20 **Mykyta Bobylyow** «Change in orientation of the Ca^{2+} sensor protein hippocalcin in its membrane-bound state as a mechanism for the development of primary dystonia» *(Department of Molecular Biophysics, Bogomoletz Institute of Physiology; Instytut Chemii Bioorganicznej Polskiej Akademii Nauk, Poznan)*

15.35 **Mykyta Bobylyow** «Collective behavior of the lipid bilayer and the role of PIP_2 in binding the neuronal Ca^{2+} sensor protein hypocalcin» *(Department of Molecular Biophysics, Bogomoletz Institute of Physiology; Instytut Chemii Bioorganicznej Polskiej Akademii Nauk, Poznan)*

15-50 **Coffee break**

16-10 **Polina Kanevska**
«Role of internal conformation in the coupled deformation of DNA» *(Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine)*

16-40 **Oleksandr Shovkoplias** «Conformational mobility of Trp128 in the EMAP II protein: molecular dynamics study» *(Taras Shevchenko National University of Kyiv)*

17-00 **Andrii Lesiuk**
«Protein Interactions with bioactive molecules and oxide nanoparticles: spectroscopic and computational studies» *(Taras Shevchenko National University of Kyiv)*

17.30 **Closing**