

Scientific workshop for students
Computational Physics of DNA
May 21-23, 2024

PROGRAM

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

Tuesday **21.05.2024**



[Sergiy Perepelytsya](#)

10-00

OPENING

**Lecture
in person**

**Molecular dynamics: from the problem of
hard spheres to the DNA macromolecule**

10-05

Bogolyubov Institute for Theoretical Physics

11-00

of the NAS of Ukraine



[Francesca Mocci](#)

**Lecture
online**

**Force fields and molecular dynamics
simulations: Applications to nucleic acids**

11-00

Department of Chemical and Geological

12-00

*Sciences, University of Cagliari (Cagliari,
Italy)*

12-00

Coffee break

12-30



[Sergey Volkov](#)

**Lecture
in person**

Conformational mechanics of DNA

*Bogolyubov Institute for Theoretical Physics
of the NAS of Ukraine*

12-30

13-30

13-30

Lunch

14-30



[Anna Shestopalova](#)

Lecture
14-30
15-30

Computational methods of structural bioinformatics in studies of the indirect mechanism of protein-nucleic recognition
O.Ya. Usikov Institute for Radiophysics and Electronics of the NAS of Ukraine.



[Tetiana Bubon](#)

Practice in person
15-30
17-00

Getting started with GROMACS and VMD program packages
Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine

Wednesday

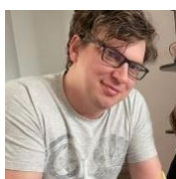
22.05.2024



[Oleksii Zdorevskyi](#)

Lecture online
10-00
11-00

Hybrid quantum-mechanics/molecular mechanics (QM/MM) simulation methods and their applications to studying charge transfer processes in redox proteins
University of Helsinki



[Tudor Vasiliu](#)

Lecture online
11-00
12-30

Using ChatGpt in molecular dynamics simulations: Applications to nucleic
Centre of Advanced Research in Bionanoconjugates and Biopolymers "Petru Poni" Institute of Macromolecular Chemistry (Iasi, Romania)

12-30
14-00

Lunch



[Tetiana Bubon](#)

Practice in person
14-00
16-00

Molecular dynamics simulations of the DNA double helix with GROMACS
Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine

Thursday

23.05.2024



[Kestutis Aidas](#)

*Lecture
online*

10-00

11-00

Modelling NMR properties of complex molecular materials by means of an integrated MD-QM/MM approach

Vilnius University



[Anna Shestopalova](#)

Lecture

11-00

12-00

Computer simulations of DNA-ligand intercalation complexes: some special features

O.Ya. Usikov Institute for Radiophysics and Electronics of the NAS of Ukraine.

12-00

12-30

Coffee break



[Tetiana Bubon](#)

*Lecture
in person*

12-30

13-30

Specific effects of alkali metal ions on the vibrational dynamics of DNA ion-hydration shell

Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine

13-30

14-30

Lunch



[Tetiana Bubon](#)

*Practice
in person*

14-30

17-00

Analyzing molecular dynamics trajectories of the DNA double helix using GROMACS and VMD

Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine

17-00

CLOSING