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CHRONICLE

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THE 2nd SCIENTIFIC WORKSHOP FOR STUDENTS "COMPUTATIONAL PHYSICS OF DNA"

The 2nd Scientific workshop for students "Computational Physics of DNA" took place on May 21-23, 2024 in Kyiv, Ukraine, at the Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine (BITP). The event was organized in a hybrid offline-online format by joint efforts of the BITP and the Kyiv Academic University (KAU). Over 30 students from various universities of Ukraine participated, including from Taras Shevchenko National University of Kyiv, the National University of Kyiv-Mohyla Academy, the National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute". Students from foreign scientific centers in Italy, Romania, and Slovakia also attended the event. The lecturers and teachers of the school were leading scientists in this field: Dr. Sci. Sergiy Perepelytsya (BITP), Professor Francesca Mocci (University of Cagliari, Italy), Dr. Sci. Sergey N. Volkov (BITP), Dr. Sci. Professor Anna Shestopalova (Institute of Radiophysics and Electronica of the NAS of Ukraine), Dr. Oleksii Zdorevskyi (University of Helsinki, Finland), Dr. Tudor Vasiliu ("Petru Poni" Institute of Macromolecular Chemistry, Romania), Professor Kęstutis Aidas (Vilnius University, Lithuania), and Tatiana Bubon (BITP).

The lectures were focused on the physics of DNA and modern methods for modeling the structure and dynamics of the macromolecule at different levels of its organization. The general overview of the methods of classical molecular dynamics (MD) simulations and their application to DNA-systems has been provided by Sergiy Perepelytsya [1]. Francesca Mocci, in her lecture, did the detailed description of the interaction potentials and modern force fields that are used in classical MD simulations of nucleic acids [2]. Sergey N. Volkov discussed physical models of the conformational mechanics of DNA, describing the experimentally observed effects of the double helix bending, overstretching, and unzipping [3]. Anna Shestopalova delivered two lectures. In the first lecture, she described the methods of structural bioinformatics in studies of the indirect mechanism of protein-nucleic recognition [4], while in the second one, the MD insights of the problem of DNA-ligand interactions [5]. Oleksii Zdorevskyi covered quantum mechanics/molecular mechanics (QM/MM) simulation methods and their applications for studying charge transfer processes in redox proteins [6]. Tudor Vasiliu's lecture was focused on the practical use of ChatGPT for various applications in MD simulations of nucleic acids [7]. Kęstutis Aidas, in his lecture, described the integrated QM/MM approach for modelling NMR spectra of complex molecular materials [8]. Tetiana Bubon presented the results on the structure and dynamics of the DNA ion-hydration shell, discussing the results of modeling the vibrational spectra of DNA in aqueous solutions using classical MD simulations [9]. The practical classes, organized by Tetiana Bubon, were

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devoted to VMD and GROMACS software packages and how to use them for doing classical MD simulations [10–12]. The computational cluster of the BITP was used during the practical classes. The lectures and practical seminars are available on the BITP YouTube channel [1–12].

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