

# NANOPHYSICS MEETS COMPUTER SIMULATIONS



## 1st annual workshop on the use of computer simulations in nanophysics

November 8, 2024

Institute for Condensed Matter Physics of NAS of Ukraine

1 Svientsitskii Street, Lviv, Ukraine

<https://icmp.lviv.ua/nanosim>

- 12:00-12:40 **Volodymyr Kapustianyuk**, Ivan Franko National University of Lviv, Lviv  
*Size effects in the ferroic nano- and microcomposites*
- 12:40-13:00 **Oleg Bovgyra**, Ivan Franko National University of Lviv, Lviv  
*First-principles study of the structural, electronic, and sensing properties of ZnO nanostructures*
- 13:00-14:30 **Lunch break**
- 14:30-15:10 **Stepan Mudry**, Ivan Franko National University of Lviv, Lviv  
*Structure of nanoparticles, studied by means of small angle X- ray scattering method*
- 15:10-15:50 **Ihor Zavaliiy**, Karpenko Physico-Mechanical Institute, Lviv  
*Hydrogenation - disordering of structure correlations for nano- and amorphous Ni-based materials*
- 15:50-16:30 **Ari Paavo Seitsonen**, ENS, Paris  
*Electronic structure calculations supporting and explaining experimental findings at surfaces: Atomistically precise nano-ribbons and molecules*
- 16:30-16:40 **Coffee break**
- 16:40-17:20 **Sergiy Minko**, University of Georgia, Athens, [presentation by zoom](#)  
*Dynamic polymer interfaces for switchable adhesion of colloidal particles*
- 17:20-17:40 **Andriy Stelmakh**, ETH, Zurich, [presentation by zoom](#)  
*Equilibrium Shapes and Surface Structures of Bare and Ligand-Capped CsPbBr<sub>3</sub> Quantum Dots*
- 17:40-18:00 **Jaroslav Hnytskyi**, ICMP, Lviv  
*Adsorption of low density lipoproteins on an azobenzene-containing polymer brush*
- 18:00-19:30 **Poster session**
- 20:00-21:00 **Conference dinner**

- 9:00-9:10 **Taras Bryk**, ICMP, Lviv  
*Interdisciplinary center for computer simulations: current status and perspectives*
- 9:10-9:50 **Maryna Bodnarchuk**, EMPA, Zurich  
*Structural and Compositional Engineering of Superlattices Comprising Halide Perovskite Nanocubes*
- 9:50-10:30 **Simon C. Boehme**, ETH, Zurich  
*Strategic use of exciton-phonon coupling in lead-halide perovskite quantum dots for quantum-light applications*
- 10:30-11:10 **Alexander Krivchikov**, Verkin Institute for Low Temperature Physics, Kharkiv  
*Low-temperature heat capacity of carbon nanotubes and anomalous dispersion of the transverse acoustic branch in the case of layer materials*
- 11:10-11:20 **Coffee break**
- 11:20-11:40 **Jaroslav Gnilitskyi**, NoviNano Lab, Lviv  
*Deciphering of femtosecond laser-induced self-organised nano/microstructures*
- 11:40-12:00 **Mykola Isaiev**, CNRS, Universite de Lorraine, Nancy, [presentation by zoom](#)  
*Molecular Dynamics Simulations of Thermophysical Properties of the Novel Materials for Green Energy Transition*

