

Computational Molecular Physics at Work

Tuesday 25 November 2025 16:30 (20 minutes)

I'll give a brief overview of computational molecular physics (CMP) techniques in my talk. They fall into two groups: Molecular Mechanics (MM) and Quantum Mechanics (QM). MM approaches use predefined analytical interatomic potentials, whereas QM approaches rely on an approximate solution of the many-electron Schrödinger equation. Likewise I'll describe few open-source CMP applications that Govorun users can utilize for their scientific work at JINR.

Presenter: Dr ИЛБЯШ, Мирослав (BLTP JINR)