Short CV:

Jure Borišek was born and raised in Slovenia, where he obtained his Master's degree in Pharmacy and Ph.D. in Biomedicine from the University of Ljubljana. He then joint prof. dr. Magistrato's group at SISSA as a postdoctoral fellow. He started his academic career in QSAR modelling using artificial neural networks, then moved to medicinal chemistry projects using various experimental and computational chemistry techniques, and now works mainly on molecular simulations of biomacromolecules. He is currently head of the Laboratory for Cheminformatics at the National Institute of Chemistry in Slovenia.

Abstract:

Research assoc. prof. dr. Jure Borišek: 'Machine learning paving a new era in molecular dynamics simulations'

Molecular dynamics (MD) simulations are a key computational chemistry technique that provide dynamic insight into the underlying atomic-level processes in the system under study. These insights not only improve our understanding of the molecular world, but also aid in the design of experiments and targeted interventions. Currently, MD is associated with several limitations, the most important of which are insufficient sampling, inadequate accuracy of the atomistic model, and challenges with proper analysis and interpretation of the obtained trajectories. Although numerous efforts have been made to address these limitations, more effective solutions are still needed. The recent development of artificial intelligence, particularly machine learning (ML), offers exciting opportunities to address the challenges of MD. In this talk I will highlight the basics of MD together with its limitations. I will outline the advancements made by ML, including the development of ML-based force fields, techniques for improved conformational space sampling, and innovative methods for trajectory analysis. Additionally, I will present the challenges and implications associated with the integration of ML and artificial intelligence. While the potential of ML-MD fusion is clearly established, further applications are needed to confirm its superiority over traditional methods.