

# 7<sup>th</sup> Users' Conference of IT4Innovations

30–31 October 2023

**10:00 – 11:00 | Registration and networking**

Monday 30 October 2023

**11:00 – 11:30 | Welcome and IT4Innovations news**

**11:30 – 12:00 | KEYNOTE I**

The first CACHE challenge: searching for hit molecules in ultra-large chemical databases  
[Pavel Polishchuk](#) | [Palacký University Olomouc](#)

**12:00 – 13:00 | Users' Talks I**

Extramedullary multiple myeloma: insights into pathogenesis and tumor microenvironment using whole exome, RNA and single-cell sequencing  
[David Žihala](#) | [University of Ostrava](#)

Quantum chemistry and machine learning for computer-aided drug design  
[Jan Řezáč](#) | [Czech Academy of Sciences](#)

Atomistic simulations of ancient ribosomes and their parts  
[Michal H. Kolář](#) | [University of Chemistry and Technology Prague](#)

**13:00 – 14:00 | Lunch & Poster Session**

**14:00 – 15:00 | Users' Talks II**

Interactions of ionizable and cell membrane lipids  
[Petra Čechová](#) | [Palacký University Olomouc](#)

Biocompatibility of carbon nanomaterials from an in-silico perspective  
[Markéta Paloncýová](#) | [Palacký University Olomouc](#)

Benchmark of time-dependent density functional theory simulations on a variety of European CPU-based supercomputers  
[Thibault J.-Y. Derrien](#) | [Czech Academy of Sciences](#)

**15:00 – 16:00 | USERS' COUNCIL**

**16:00 – 16:30 | Coffee Break**

**16:30 – 17:00 | KEYNOTE II**

Cinematic visualization of large scientific data sets  
[Markéta Faltýnková](#) | [IT4Innovations](#)

**17:00 – 18:20 | Users' Talks III**

Karolina system energy efficiency optimization  
[Ondřej Vysocký](#) | [IT4Innovations](#)

A first principles study of structural and optoelectronic properties and photocatalytic performance of GeC-MX<sub>2</sub> (M = Mo and W; X= S and Se) van der Waals heterostructures  
[Tahir Wahab](#) | [Czech Technical University in Prague](#)

Employing supercomputers to determine the local structure of framework and extra-framework species and to subsequently evaluate their NMR parameters for comparison with experiments  
[Štěpán Sklenák](#) | [Czech Academy of Sciences](#)

Generating coupled cluster code for modern distributed memory tensor software  
[Jan Brandejs](#) | [Laboratoire de Chimie et Physique Quantiques](#)

**18:20 - 21:00 | Conference Dinner & Poster Session**

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## 09:00 – 09:30 | KEYNOTE III

Plasma shutter for laser-driven ion acceleration and spiral pulse generation  
[Martin Matys](#) | [ELI Beamlines](#)

Tuesday 31 October 2023

## 09:30 – 10:50 | Users' Talks IV

Numerical simulations at Karolina for advancing research at ELI NP  
[Vojtěch Horný](#) | [Extreme Light Infrastructure Nuclear Physics](#)

Testing the accuracy of random-phase approximation for molecular solids  
[Jiří Klimeš](#) | [Charles University in Prague](#)

Quantum mechanical insights into the optical properties of carbon dots  
[Miroslav Medved'](#) | [Palacký University Olomouc](#)

MoS<sub>2</sub> crystallization via reactive molecular dynamics simulations  
[Iliia Ponomarev](#) | [Czech Technical University in Prague](#)

## 10:50 – 11:00 | Coffee Break

## 11:00 – 12:00 | Users' Talks V

Interatomic interactions in the vicinity of lattice defects in intermetallics  
[Martin Zelený](#) | [Brno University of Technology](#)

Magneto-elastic properties calculation via computational high-throughput approach  
[Dominik Legut](#) | [IT4Innovations](#)

Structural tuning of band gap in doped diamonds  
[Matúš Kaintz](#) | [Czech Technical University in Prague](#)

## 12:00 – 13:00 | Lunch