

IT4Innovations,  
Czech National Supercomputing Centre  
Ostrava, CZ

# International workshop devoted to magnetism, spin-orbit coupling, and lattice dynamics for 3D and 2D systems

within the CZ-SK *Influence of thermoelectrical effects on spin-orbit torques in 2D van der Waals materials* project No. LUASK22099 supported by Ministry of Education, Youth, and Sports of the Czech Republic

November 22th 2023

## Dopolední program:

9:55 D. Legut (IT4I) - Introduction

10:00 D. Legut (IT4I)- Thermal conductivity from first principles

10:20 M. Gmitra (UPJS) - Proximity-induced spin-orbit and magnetic exchange coupling in graphene

10:40 I. Korniienko (IT4I) - Theoretical analysis of the design of THz radiation spin-based sensors

11:00 J. Mních (UPJS) - Magnetic properties of monolayer and bilayer NiI<sub>2</sub>

11:20 Jan Priessnitz (IT4I) - High-throughput calculation of magnetic exchange interactions using DFT

11:40 M. Rassekh (UPJS) - Proximity-Induced Spin Currents and Spin-Orbit Torques in Graphene on 1T-TaS<sub>2</sub>

Oběd: 12:00-13:40

## Odpolední program:

13:40 S. Pastukh (INP) - Anharmonicity and structural phase transition in the Mott insulator Cu<sub>2</sub>P<sub>2</sub>O<sub>7</sub>

14:00 T. Moško (UPJS) - Electronic structure study of intercalated monolayers and their van-der-Waals heterostructures

14:20 M. Milivojević - Spin-Orbit Proximity Effect in P-WSe<sub>2</sub> and WSe<sub>2</sub>-P-WSe<sub>2</sub> Heterostructures

**Panel discussion: 14:40-16:30** Devoted to the progress, plan of the project and strategies how to make it more synergic for both teams.

16:30 - 17:00 D. Legut - Overview of the HPC capabilities at IT4Innovations