

CEIPEX BUT TOPIC 15

Položka / Field	Obsah / Content
CEIPEX RESEARCH TOPIC LEVEL 1	Advanced Nano & Micro technologies
CEIPEX RESEARCH TOPIC LEVEL 2	Magneto-optical & THz spectroscopy
NAME OF THE RESEARCH GROUP	Magneto-optical & THz spectroscopy (RG-1-12)
SUPERVISOR	Dr. Petr Neugebauer
POTENTIAL CO-SUPERVISOR	Dr. Ivan Šalitroš
PROPOSED RESEARCH TOPIC TITLE	Theoretical investigation of magnetic molecules supported on 2D materials and nanostructures using advanced quantum-chemical and molecular-modelling methods
RESEARCH TOPIC DESCRIPTION	The integration of magnetic molecules with two-dimensional materials and other nanostructured systems offers new opportunities for the development of functional materials with tailored electronic and magnetic properties. This research topic focuses on the theoretical design and characterization of such hybrid systems using advanced computational methods. The candidate will: • Participate in research projects investigating the magnetic properties of molecules supported on 2D materials and other nanomaterials. • Design and screen new molecular and nanostructured materials at the theoretical level using density functional theory calculations. • Calculate and interpret the magnetic properties of the investigated systems. • Characterize the electronic structure, chemical bonding and dynamics of nanostructures and 2D materials using advanced theoretical methods, including DFT, ab initio molecular dynamics, QTAIM and multireference calculations. • Perform computational calculations in high-performance computing environments and use Python for computational workflows and data analysis. • Process and interpret computational data and, where relevant, correlate theoretical predictions with experimental results, including 4D-STEM datasets. • Publish the obtained results in peer-reviewed scientific journals. • Collaborate closely with other members of the research group and contribute to interdisciplinary research activities at CEITEC BUT.
KEYWORDS	2D materials, nanomaterials, magnetism, advanced computational methods
WEBPAGE OF THE RESEARCH GROUP	https://www.ceitec.eu/magneto-optical-and-thz-spectroscopy/rg259