Charles University

XIX. Call for the Junior Fund, 2026

Proposal for a research project

Faculty/institute/unit of CU:	Faculty of Science
Department:	Department of Physical and Macromolecular chemistry
Research project title:	Machine Learning-Driven Materials Design For Functional Oxides
Project description:	This position offers the candidate the opportunity to join a dynamic team of researchers at the forefront of *in silico* atomistic modelling of solid oxidic nano-materials. The project combines method development and application towards bottom-up materials design in the areas of sustainable energy and energy storage, supported by international collaborations and European research networks. You will push the boundaries of computational materials chemistry for selected systems, and bridge the materials gap between experiment and theory. Specifically the project consists of three main themes: 1. **Development and application of state of the art ML-Interatomic Potentials (MLIP)** to advance atomistic modelling under realistic conditions of functional solid oxide materials of industrial importance, including i) photocatalytic Cu_2O surfaces, and ii) battery cathode materials. A modelling pipeline will be deployed involving unbiased global structure optimisation, accelerated dynamics simulations of system evolution and structural refinement. **2. Diffusion modelling under field/concentration-induced non-equilibrium conditions.** You will advance the field by introducing field and concentration effects to study the dynamics of ion diffusion and surface reconstruction at photocatalytic interfaces under *operando* conditions. You will develop kinetic networks using discrete path sampling (hybrid Eigenvector-Following) and biased dynamical approaches (metadynamics/umbrella sampling), to link the underlying nature of the free energy surface to dynamical properties, in order to optimise material functionality and design next generation functional oxides. **Theoretical Characterisation and Experimental Confirmation.** Model evaluation and comparison will be

Ovocný trh 560/5, 116 36 Praha 1
phone: (+420) 224 491 307
www.cuni.cz
IČO: 00216208 DIČ: CZ00216208

	provided via direct two-way collaboration with experimental partners, in particular via XPS, LEED-IV, conductivity measurement and solid state NMR spectroscopy. You will calculate ion mobility/conductivity measurements, and confirm structural models via ML-based tensorial NMR spectroscopic models already developed within the group. Networking and collaboration: MLIPs & ML-based property predictors: V. Deringer (Oxford, UK); R. Gómez-Bombarelli (MIT, US); C. Bornes (CICECO Aveiro, PT); A.M. Elena (STFC, UK) ML-accelerated structure and reaction sampling: D. Wales (Cambridge, UK); B. Slater (UCL, UK); A. Fortunelli (Pisa, IT) Application-driven: G. Parkinson (TU Wien, AT) Relevant project publications: 1. Nat. Commun., 2024, doi: 10.1038/s41467-024-48609-2 2. J. Catal., 2025, doi: 10.1016/j.jcat.2025.116533
What do we offer?	Two-year fixed-term position which can be further extended if additional funds become available.
Profile of an ideal candidate:	The ideal candidate will have a recent PhD in the fields of physics, chemistry or material science, with experience in quantum chemical calculations (required) and machine learning approaches (preferred). (S)he will be able to demonstrate independent research work, critical analysis and project management skills. Preferred: experience and interest in project and student supervision.
Position available from:	October 1, 2026
Workplace location:	Hlavova 8, Prague 2
Supervisor(s):	Christopher J. Heard, PhD.
E-mail:	heardc@natur.cuni.cz
Application deadline:	May 15, 2026
Applicants must submit required documents to:	Christopher J. Heard, PhD.