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:	Developing machine learning tools for reactive atomistic material modelling
Project description:	This position offers an opportunity to advance computational material chemistry through machine learning (ML), focusing on three key areas: **1) ML Interatomic Potentials (MLIPs).** You'll develop and refine data-efficient MLIPs based on equivariant architectures (MACE), leveraging our GPU-accelerated KDE uncertainty quantification framework for active learning and teacher–student distillation for generating fast, transferable models. Transfer learning and delta-learning broaden applicability across compositions and material classes. **2) ML-Driven Property Prediction.** The role involves predicting tensorial properties — in particular full NMR tensors (chemical shifts, quadrupolar parameters, J-couplings) via equivariant GNNs — enabling direct comparison with experimental solid-state NMR spectra. The pipeline extends to Raman and IR spectra, with the goal of building a unified multi-spectral prediction framework. **3) Advanced (ML-Accelerated) Sampling.** You'll develop ML-accelerated tools for global structure search (minima hopping, basin hopping with material-specific move classes), reaction network mapping via the OPTIM toolkit (single- and double-ended transition-state searches → disconnectivity graphs → adaptive kMC), and enhanced sampling for free energy surfaces (automated umbrella sampling, ML-based collective variables). The work builds on a validated computational platform tested on porous aluminosilicate systems (zeolites), with natural application extensions to material synthesis, cation exchange in layered materials, and catalyst design. This is a chance to contribute cutting-edge research at the ML–chemistry interface

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	within an internationally connected 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); T. Verstraelen (Ghent, BE); C. Chizallet (IFPEN, FR); B. Slater (UCL, UK) Application-driven: J.D. Rimer (Houston, US); J. Rocha ((CICECO Aveiro, PT) Relevant project publications: 1. Nat. Commun., 2024, doi: 10.1038/s41467-024-48609-2 2. Digital Discovery, 2025, doi: 10.1039/D4DD00306C 3. J. Phys. Chem. Lett., 2025, doi: 10.1021/acs.jpclett.5c02595 4. arXiv, 2026, doi: 10.48550/arXiv.2603.22268 (tensorial GNN NMR predictor)
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 holds a PhD in computational chemistry, physics, materials science, or a related field, with a solid background in machine learning and atomistic simulations. Working knowledge of relevant ML or MD frameworks is expected, and a reasonable publication record demonstrating scientific curiosity and rigor is valued. Strong motivation to work at the ML–chemistry interface and to collaborate within an international research network is key.
Position available from:	October 1, 2026
Workplace location:	Hlavova 8, Prague 2
Supervisor(s):	doc. RNDr. Lukáš Grajciar, PhD.
E-mail:	lukas.grajciar@natur.cuni.cz
Application deadline:	May 15, 2026
Applicants must submit required documents to:	doc. RNDr. Lukáš Grajciar, PhD.