Charles University

XIX. Call for the Junior Fund, 2026

Faculty Proposal for a Research Project

Faculty:	Mathematics and Physics
Department:	Chemical Physics and Optics
Research project title	Machine learning of interatomic potentials for force field parameterization in nanotubular clays
Project description	To derive force fields parameters for solving the structures of clay minerals like haloysite and immogolite, the use of machine learning potentials (MLPs) is a suitable method. MLPs can be used to predict interatomic potentials with less computational costs than density function theory methods and, with the use of current AI, lead to a more accurate determination of interatomic parameters and increase their influence on the accuracy of force field parameters. Some limitations remain, such as the description of long-range interactions that will be included. The project focuses on nanotubular clays as a general large structure that will be parametrized for atoms present in their inorganic layers. Current force fields are not able to keep this structure stable without constraints. Second, we will focus on the positions of individual atoms and their close surroundings to create small models that will be used for the parametrization training set for the most accurate interatomic parameters.
What do we offer?	Two-year position, working in research group focused on molecular simulations, cooperation with experimental laboratories in the Czech and Europe. Mobility outside Europe.
Profile of an ideal candidate:	Ph.D. in material science or chemistry, knowledge of force field calculations, clay minerals, Python. Experience with simulation software Gromacs, LAMMPS. Linux and high performance computing.
Position available from:	October 1, 2026
Workplace location:	Department of Chemical Physics and Optics
Supervisor(s):	Miroslav Pospíšil
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Application deadline:	May 18, 2026

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