



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:	Modelling protein solutions in membrane separation processes - from simple patchy colloids to realistic representation of proteins.
Project description:	<p>We aim to create and validate a novel coarse-grained modelling approach for predicting acid-base equilibria in protein solutions separated from a buffer by a semi-permeable membrane. Such predictive modelling is crucial for optimising industrial separation processes like dialysis or ultra/dia-filtration. Models based on the mean-field approximation, commonly used in the industry, sometimes fail to predict the charge on proteins and the pH in the protein solution because they do not account for the irregular shapes of proteins, their charge distribution and protein-protein interactions. By accounting for these factors, our simulations will not only improve the prediction of pH, protein charge and ion partitioning but also enable predicting phase separation and precipitation as a function of pH, which is impossible with current models. We will validate our modelling using dialysis experiments on well-known proteins. If successful, our approach will enhance the fundamental physico-chemical understanding needed to improve optimization of industrial processes.</p> <p>The goal of the project is to develop suitable coarse-grained simulation models for studying acid-base equilibria in protein solutions, suitable also for modeling of phase separation and precipitation at various pH values. The goals include benchmarking these models against well-defined experiments.</p> <p>Profile of a perfect candidate:</p> <ul style="list-style-type: none">• Proficient in Thermodynamics, Statistical Mechanics, and Physical Chemistry or Polymer Physics• Experienced in coarse-grained or all-atom simulations of polymers• Experienced in using python and grid computing <p>Please, address any questions to peter.kosovan@natur.cuni.cz</p>



What do we offer?	Two-year fixed-term position which can be further extended if additional funds become available.
Profile of an ideal candidate:	<ul style="list-style-type: none"> ● Proficient in Thermodynamics, Statistical Mechanics, and Physical Chemistry or Polymer Physics ● Experienced in coarse-grained or all-atom simulations of polymers ● Experienced in using python and grid computing ● Capable of conducting research independently
Position available from:	October 1, 2026
Workplace location:	Hlavova 8, Prague 2
Supervisor(s):	Doc. RNDr. Peter Košovan, PhD
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Phone:	+420 221 951 029
Application deadline:	May 15, 2026
Applicants must submit required documents to:	Doc. RNDr. Peter Košovan, PhD