



NARODOWE CENTRUM NAUKI



HR EXCELLENCE IN RESEARCH

## PhD Position

# Computational studies of diffusion in crowded environments inside living cells

**Background.** Biochemistry of life, on the cellular level, is driven by two elementary physical processes: Diffusion of macromolecules and metabolites, and enzyme-catalyzed conversion of metabolites (the latter will not be considered in this project). The cytoplasm, the cellular interior where diffusion and reactions take place, is overcrowded with molecules, hence physicochemical conditions inside the cells differ significantly from what is used in a typical laboratory system. In particular, self-diffusion coefficients of proteins and metabolites decrease significantly, and the diffusion process can anomalously slow-down under certain conditions. Since diffusion determines essentially the kinetics of many cellular processes, its study is of vital importance for life sciences and biotechnological applications.

**Project description.** The successful candidate will conduct simulation studies of macromolecular diffusion and metabolic transport in crowded environments akin of the inside of living cells. The project consists of three parts. In the first part the effect of macromolecular shapes and sizes will be studied in order to understand recent experimental results by Profesor Fitter group (Aachen University), which show a nontrivial dependence of diffusion on the shapes of macromolecules. The second part deals with the metabolism-dependent diffusion. Recent experiments show a tremendous effect of the cell metabolism on the diffusion of large macromolecules, which slow down dramatically when the cell metabolism is suppressed. Computer simulations will be used to understand and rationalize this effect. In the third part the focus will be on transport properties of metabolites, with the aim to develop a consistent method for determining the transport diffusion coefficients for future spatially-resolved whole-cell simulations.

**What we offer.** We offer a NCN-funded 3 year PhD position with a competitive stipend of more than 1000 Euro (depending on the performance), with the possibility to prolong for another year. The project will be carried out in the Institute of Physical Chemistry (ICP) located in a vibrant and fast developing city of Warsaw. The ICP is one of the leading research institutes in Poland and among the best in Central and East Europe. The project will be conducted in collaboration with RWTH (Aachen University, Germany) and Forschungszentrum Jülich (the largest research center in Europe). The successful candidate will have to pass an entry exam for (or be on) the ICP doctoral studies (see <http://ichf.edu.pl/msd/indexen.html> for details), with the possibility to receive an *additional stipend/salary* from ICP.

**Requirements.** We are looking for an enthusiastic and motivated young scientist with a background in physics, theoretical chemistry, biology or related fields of study. Experience in C/C++, Linux, HPC and molecular simulations is highly desirable, as well as good communication skills and strong interest in multidisciplinary research.

**Dates.** Deadline for applications: 15th June. Decision: 15th July. Start date: 1st November 2018.

**How to apply.** Send your CV and the statement of interest to S. Kondrat ([skondrat@ichf.edu.pl](mailto:skondrat@ichf.edu.pl) and [svyatoslav.kondrat@gmail.com](mailto:svyatoslav.kondrat@gmail.com)). Informal inquiries are welcome.