

## **Project 4.1 Molecular dynamics of systems of the intrinsically disordered proteins (theoretical)**

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**Institute:** IF PAN

**Unit:** SL-4

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### **Background:**

Theoretical and computational biophysics/biochemistry used to understand proteinaceous liquid droplets

### **Aim:**

In recent years, there has been a tremendous interest in the properties of the intrinsically disordered proteins, primarily in the context of the neurodegenerative diseases. Oftentimes the aqueous solutions of these proteins undergo liquid-liquid phase transitions that result in the formations of the proteinaceous droplets. The droplets act as membraneless organelles that provide a more concentrated environment to perform various biological functions. The idea of the project is to use simulations to derive phase diagrams of such solutions and to understand how such droplets form and what are their properties. This project is done in parallel to the European PathoGelTrap H2020 grant that is focused on involving such droplets of chimeric proteins in the fish aquaculture to capture toxins that plague breeding of salmon and other species. The modelling will be based both on all-atom and coarse-grained simulations. The latter will be based on the available in-house programs.

### **Requirements:**

- Research experience in theoretical physics, chemistry or computer science.
- Experience with biological issues
- Master's degree in physics, chemistry, biophysics (or an equivalent degrees).
- Sufficient proficiency in the English language that scientific interaction is not hindered.

### **Funding:**

e.g.

Scholarship: grant funding of 4500 PLN per month, before subtracting obligatory employer and employee social security contributions (~15%), for 18 months. Afterwards, standard Polish PhD scholarship (about 2100 PLN/month net in years 1-2, 3240 PLN/month net in years 3-4).

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