

# Postdoctoral position for a junior scientist in the Laboratory of Molecular Modeling, Faculty of Chemistry, University of Gdańsk, Poland

**Project title:** “Correlated mean-field interactions propagated along polypeptide chain as a key to understanding the structure formation, dynamics, and allostery of proteins and physics-based modeling thereof”

**Project leader:** prof. dr hab. Józef Adam Liwo

**Position name:** Postdoctoral Associate (adiunkt naukowy)

## Requirements:

1. Ph.D. degree in Chemistry, Physics, Biology, Biotechnology or related disciplines or evidence that the degree will be conferred by the start of the employment. **By the rules of the grants agency (NCN), the date of conferring the Ph.D. degree must not be earlier than 7 years before the start of the employment financed from the project.**
2. Command of English sufficient to read scientific papers and for communication.
3. Knowledge of molecular quantum mechanics, statistical mechanics, and methods of computational chemistry. Experience in force-field development is desirable.
4. Experience in running and analysing the results of molecular dynamics simulation. Experience in metadynamics and extensions of molecular dynamics (replica exchange) is desirable.
5. Knowledge of statistical methods of data analysis. Familiarity with Principal Component Analysis and machine learning is desirable.
6. Knowledge of the basic principles of protein structure organization.
7. Ability to work with UNIX-operated workstations at least at the medium-advanced level, including the ability to write UNIX scripts. Literacy in Fortran/C/C++ is desirable.
8. Reliability and ability to solve scientific problems independently.

## Project information:

Proteins are macromolecules with highly organized structures and highly concerted dynamics, which are manifested as allosteric communication enabling, e.g., signal transduction, and in motility inherent in molecular motors. Very accurate methods based on Artificial Intelligence, such as AlphaFold in the first place, have recently been developed for modeling protein structures but we are still far from understanding how interatomic interactions converge into certain structural patterns and concerted motions. The bottom-up coarse-grained approaches can be used to find the solution of this problem.

In our laboratory, we are developing the UNRES coarse-grained model of proteins, in which a polypeptide chain is represented by the  $\alpha$ -carbon trace with united peptide groups

and united side chains as interaction sites. This model is efficient in simulating protein structure and dynamics, enabling 1000-fold extension of the simulation time-scales compared to all-atom approaches. The physical basis of UNRES enables us also to interpret the components of the coarse-grained force field as pre-determined blocks of interactions that organize protein structure and dynamics. When all-atom approaches are used, such organized patterns could be discerned only by applying Principal Component Analysis and similar techniques. Recently, we discovered new coarse-grained terms that correspond to long-range collective interactions along extended and helical sections of polypeptide chains.

The aim of this project is (i) to determine how long-range correlations between amino-acid residues sitting on distant parts of the polypeptide chain, which do not interact with each other directly contribute to the formation of protein tertiary structure, (ii) to use the obtained results in enriching the coarse-grained UNRES force field in the respective effective energy terms, which will presumably enhance its power to correctly predict global complicated folds, (iii) to investigate if and how these correlations contribute to the protein dynamics, especially to allosteric interaction and to the exceptional performance of molecular rotatory motors.

### **Tasks assigned to the position:**

1. Parameterization of the already derived multi-torsional terms and their implementation in UNRES.
2. Derivation of the site-based terms accounting for along-sequence correlation and analyzing Protein Data Bank (PDB) and AlphaFold database to find these correlations in protein structures and parameterization of these terms.
3. Calibration of the UNRES force field with the the new terms.
4. Testing the performance of the enhanced UNRES to model complex protein folds, including the participation in the Community Wide Experiments on the Critical Assessment of Techniques for Protein Structure Prediction (CASP).

### **Conditions of employment:**

1. Full-time 1-year job contract, extendable to 2 years.
2. Gross-gross salary: 12000 PLN. The gross-gross salary includes health insurance and pension plan.
3. Approximate date of employment start: January 1, 2025, possibly earlier.

### **Application package must include the following:**

1. Cover letter.
2. CV including the list of publications.
3. A copy of Ph.D. diploma or documented proof that the applicant will obtain the Ph.D. degree (scan/electronic version acceptable).

4. At least one recommendation letter from a previous supervisor; applicants who apply for the first postdoc position must supply the recommendation letter from the Ph.D. work supervisor. **The recommendation letter has to be emailed by the recommended directly to adam.liwo@ug.edu.pl**

**The applicant is obliged to submit, together with the documents listed above, the information clause (agreement to process personal data for the purpose of application), which can be downloaded from the web page of the University of Gdańsk or obtained from the project leader.**

The application package can be submitted in person to the Office of the Dean of the Faculty of Chemistry, University of Gdańsk, ul. Wita Stwosza 63, 80-308 Gdańsk, Poland, mailed to Prof. J.A. Liwo to the above address or, preferably, emailed to Prof. J.A. Liwo to **adam.liwo@ug.edu.pl**; the cover letter can be included in the email body, scans of the other documents attached to the email.

Selected candidates will be invited for an interview, which will be conducted in person at the Faculty of Chemistry, University of Gdańsk or online. The candidates will be notified of the time and form of the interview by email.

Any questions should be sent by email to Prof. Liwo at **adam.liwo@ug.edu.pl** or **adam.liwo@gmail.com**.

Applications should be submitted by **September 30, 2024**. Applications submitted after this date will be considered until the candidate for the position is finally selected.