



# Institute of Physics of the Polish Academy of Sciences

## Scholarship for a PhD Student



Job ID: #JOB 21/2021

### Job Description

**Job Title:** PhD student – scholarship holder

**Job Summary:**

Computational studies of disulfide bonds in proteins

**Job Description:**

The student will join the group under the supervision of dr Paweł Krupa and prof. dr hab. Mai Suan Li, working on the NCN funded project “Computational studies of the disulfide-bond role in proteins”. The aim of the PhD project are computational studies of disulfide bonds in proteins using all-atom and coarse-grained force fields. This includes:

- \* Development and improvements of potentials describing disulfide bonds in proteins.
- \* Use of the obtained potentials to study biologically important proteins, such as ribonuclease A and lipid transfer proteins.
- \* Molecular dynamics simulations (conventional, replica exchange, steered).
- \* Description of the role of disulfide bonds with possible explanation of the diseases caused by some of the studied proteins.

In coarse-grained part, we will collaborate with the developers of coarse-grained UNRES force field – group of prof. Adam Liwo from University of Gdańsk.

Requirements:

Candidates are expected to possess at least basic skills and knowledge of:

- Computational methods in biophysics (especially molecular dynamics simulations)
- Biomacromolecules, especially proteins
- Very good English in writing, reading and speaking
- Ability to write scientific publications in English
- Ability to write simple scripts and computer programs
- To be employed, the candidate must be accepted into the PhD school in which the Institute of Physics participates. Applications for the position are through recruitment to the School, online at <http://warsaw4phd.eu> .

**Main research field:** Physics

**Sub Research Field:** Computational biophysics

**Career Stage:** Early stage researcher or 0-4 yrs (Post-graduate)

**Research Profile** ([details](#)): First Stage Researcher (R1)

**Type of Contract:** Fixed term (30 months) with possible extension.

**Status:** Full-time

**Salary:** 4675 PLN per month (grant funding, before obligatory social security contributions).

## Contact

More information can be obtained from the grant PI:

Paweł Krupa (e-mail: [pkrupa@ifpan.edu.pl](mailto:pkrupa@ifpan.edu.pl))

## Application details

**Application deadline: 06.06.2021** Later applications will not be considered.

### Required materials:

- Scientific CV
- Cover letter
- Scan of MsC diploma or equivalent (or an explanation of when one is expected)
- Academic record (for finalized semesters)
- A recommendation letter by an academic, or their contact email.

All materials should be submitted in electronic form by application to the PhD school <http://warsaw4phd.eu>, choosing the project: "*Computational studies of disulfide bonds*". (The application system will be active from 24 May 2021).