



KSB 8/2024

Kraków, 10.06.2024

## Research specialist in the Adsorption group

- Employer: Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences, Krakow, Poland
- Research field:  
Chemistry > computational chemistry, molecular chemistry, physical chemistry
- Researcher profile: R2
- Deadline for applications: 21.06.2024, 16:00 pm GTM+1
- Place: Poland, Lublin
- Type of Contract: temporary
- Job Status: Full-time
- Working hours/week: 40
- Start of employment: 01.07.2024
- Key Words: carbohydrates, computer simulations, force fields, molecular dynamics.

Jerzy Haber Institute of Catalysis and Surface Chemistry PAS invites applications for a Research Specialist in the Adsorption group. The candidates who meet the conditions stated in the act "Ustawa o Polskiej Akademii Nauk" dated 30 April 2010 (Dz.U. 2018 poz. 1475 z póź. zm.), art 89. Ust. 5 for the position of Research Specialist are encouraged to apply for the position.

The candidate will participate in research conducted within the Adsorption group concerning the parametrization of coarse-grained force fields from the MARTINI family describing the behavior of carbohydrates as part of the research project OPUS 18: According to the abbreviated project description: "The main goal of the project is to create computational tools for the effective study of carbohydrate behavior and systems containing carbohydrates through molecular dynamics simulation. These tools will have the character of so-called force fields, i.e., sets of parameters approximating the interactions that occur in real systems. (...) We want to focus on so-called coarse-grained models, which are based on a simplified representation of molecules, introducing pseudo-atoms simulating the behavior of groups of real atoms. (...) We intend to create a coherent set of parameters covering a range of natural carbohydrates with various functionalizations, different types of glycosidic bonds, possible chain branches, etc. The aforementioned parameters will be compatible with those already existing and dedicated to other types of biomolecules (proteins, lipids, nucleic acids...) (...)."



In particular, the Specialist's responsibilities will include:

- Conducting simulations of a series of biomolecular systems using the molecular dynamics method at the all-atom and coarse-grained levels;
- Analyzing collected data and interpreting the results of the mentioned simulations with a focus on conformational and thermodynamic properties;
- Developing tools (scripts) for automating procedures;
- Preparing publications for high-impact factor journals;
- Reviewing scientific literature.

### Required education:

The candidate should hold a doctoral degree in the field of chemistry, physics, or related disciplines.

### Skills/qualifications:

- Doctoral degree in the field of chemistry, physics, or related disciplines;
- Proficiency in physical chemistry, chemical physics, or theoretical chemistry;
- Knowledge of the English language;
- Experience in preparing scientific reports and publications in English, confirmed by a leading role in scientific publications;
- Ability to work independently in scientific research;
- Experience in molecular modeling and basic programming skills;
- The candidate must meet the requirements specified in the NCN regulations governing the principles of employment for the postdoctoral position in the OPUS competition (18th edition).

### Specific requirements:

1. An application.
2. Completed and signed “Consent to the processing of personal data for the needs necessary to carry out the recruitment process” in accordance with the Act of 29 August 1997 on the protection of personal data (t.j. Dz. U. z 2016 r. poz. 922, z 2018 r. poz. 138, 723.) [[FORM](#)] and “Information obligations – recruitment of a perspective employee/collaborators” confirming acquainting with its content [[FORM](#)].
3. A copy of scientific degree certificate.
4. Full CV (including information on maternal leaves, voluntary work and periods of work in the industry).



5. At least one opinion on the Candidate given by an independent researcher.
6. List of scientific achievements (scientific papers, patent, patent applications, grants, etc.).
7. The Candidate's report on his/her scientific interests and research aims (an A4 page).

### Languages:

Good command of the English language in speech and writing.

### Research experience:

4-10 years of experience in research in the field of physical chemistry, chemical physics, or related areas.

### Additional information:

#### Remuneration:

The gross salary will amount to 10,000 PLN per month (gross).

#### Eligibility criteria:

- Documented experience in conducting scientific research in theoretical chemistry, physical chemistry, or related fields, confirmed by a list of publications in journals from the Journal Citation Reports list (0-10 points). Minimum required points: 3;
- Knowledge of basic programming (python, awk, bash, or other scripting language) and the Linux system (0-5 points). Minimum required points: 2;
- Familiarity with computational techniques used to describe biomolecular systems (especially molecular dynamics): (0-10 points). Minimum required points: 3.

#### Selection process:

Applications should be sent in electronic form to: sekretariat@ikifp.edu.pl with the subject title „Adsorption KSB 8/2024”

Deadline for applications: **21.06.2024 at 16:00 pm GTM+1**. The competition will be settled by **27.06.2024**. The candidates will be notified of the results.

The employment will be proceeded with accordance to the rules of Labour Code for 24 months.

#### Additional information:

The Institute has been adapted to the needs of the disabled. The Institute does not provide accommodation. The recruitment process is conducted according to [OTM-R policy](#).