



KSN 1/2023

Kraków, 12.01.2023

Assistant in the group of Theoretical and Experimental Biocatalysis

- Employer: Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences, Krakow, Poland
- Research field:
 - computational biochemistry, molecular dynamics simulations, QM/MM studies on reaction mechanisms of metalloenzymes, computational enzyme re-design
- Researcher profile: R2
- Deadline for applications: 13.02.2023, 3:00 pm GTM+1
- Place: Poland, Kraków
- Type of Contract: 18 months
- Job Status: Full-time
- Working hours/week: 40
- Start of employment: 01.05.2022
- Key Words: QM/MM, DFT, MD, metalloenzymes

Jerzy Haber Institute of Catalysis and Surface Chemistry PAS invites applications for an Assistant in the Theoretical and Experimental Biocatalysis 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. 4 for the position of Assistant are encouraged to apply for the position. The Assistant will be involved in the implementation of research statutory tasks as well she/he will work in the NewCat project.

The Candidate will take part in research conducted by the group of Theoretical and Experimental Biocatalysis, which focus on modeling of the structure of enzyme-substrate complexes using molecular dynamics methods (native forms and mutants) for enzymes from the group of non-heme iron-dependent enzymes and copper-dependent oxygenases. She/he will study the reaction pathways of these enzymes using QM/MM methods and will rationally redesign these enzymes in silico.

In particular the Assistant will be responsible for:

- conducting simulations using the molecular dynamics method
- study of reaction mechanisms using QM/MM methods
- rational redesign of enzymes in silico
- development of scripts in Python3
- preparation of scientific publications, presentation of results at conferences
- taking care of interns and doctoral students



Instytut Katalizy i Fizykochemii Powierzchni
im. Jerzego Habera
Polskiej Akademii Nauk



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Required education:

PhD in chemistry or biology

Skills/qualifications:

- experience in computational MD and QM/MM studies on the mechanisms of reactions catalyzed by metalloenzymes, documented by publications from the JCR list (0-10 pts). Minimum number of points required. 3.
- experience in redesigning enzymes in silico (0-10 pts)
- experience in programming in Python (0-5 pts).

The minimum number of points of the successful Candidate: 10.

Specific requirements:

1. An application.
2. “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](#)] (both documents filled and signed by the Candidate);
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. Copies of 3 best publications connected to the topic of the call.
8. The Candidate’s report on his/her scientific interests and research aims (an A4 page).

Languages:

English

Research experience:

4-10 years



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Additional information:

Remuneration:

The gross salary will be at least **4000 PLN/month** (roughly **850 Euro/month**) depending on the Candidate's experience.

Eligibility criteria:

- Doctoral degree in the discipline of chemical or biological sciences
- Documented achievements confirmed by publications from the JRC list or patents.

Selection process:

Applications should be sent in electronic form to: sekretariat@ikifp.edu.pl with the subject title „Assistant BTiE_KSN 1/2023”

Deadline for applications: **13.02.2023 at 3:00 pm GTM+1**. The competition will be settled by **27.02.2023**. The candidates will be notified of the results.

The employment will be proceeded with accordance to the rules of Labour Code for 18 months.

Additional information:

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