

INFORMATION ABOUT THE COMPETITION

Position name: Research associate/visiting researcher in computational chemistry

Field: Exact and natural sciences

Discipline: chemical sciences

Reference no.: AD2/W3/01/2024

Place of work: Wrocław

Type of contract: Temporary

Working time: Full-time

Faculty/Unit/Organizational unit: Faculty of Chemistry/ Wrocław University of Science and Technology

Type of position: Visiting Researcher/Research Associate in the project SONATA BIS 12, UMO-2022/46/E/ST4/00377

Research position profile: R2

Deadline for submitting applications to participate in the competition: by 02.02.2024, until 3.00 pm

Announcement expiration date: 02.02.2024, 3.00 pm

Deadline for the conclusion of the competition: 09.02.2024

Planned date of employment: April-July 2024

Period of employment and remuneration: 12 months (possible extension to full 36 months of employment), approx. **9600,00 PLN** gross (plus 13th salary and employee capital plan),

Position description:

- The Faculty of Chemistry of the Wrocław University of Science and Technology is looking for a candidate for the position of research assistant professor/visiting researcher in computational chemistry for the SONATA BIS 12 project entitled "Deciphering RNA self-replication with quantum chemistry and machine learning" led by Dr. Rafał Szabla. This project focuses on understanding the mechanistic aspects of nonenzymatic RNA self-replication using methods of molecular dynamics and quantum chemistry. In particular, the planned position is aimed at training machine learning potentials for the simulations of nucleic acids based on accurate quantum chemical data. The successful candidate will use existing models used for the generation of neural network potentials, such as SpookyNet and PhysNet and will be involved in further development of computational protocols within these framework. The funding eligibility criteria limit the maximum experience after obtaining the first PhD degree to 7 years (counted by considering the year of graduation and the year of employment in the project). This period can be extended by documented periods of long-term sickness leave or parental leave. In the case of female applicants this period can be extended by 18 months for every born or adopted child if this form of demonstrating career breaks is more beneficial (in accordance with Annex No. 2 to the Regulations for granting funds for the implementation of tasks financed by the National Science Center Poland as research projects, specified by the resolution of the NCN Council No. 60/2022 of June 9, 2022).

Responsibilities:

- Generation of training sets and performing accurate quantum chemical calculations for biomolecular fragments.

- Training and testing machine learning potentials for the simulation of nucleic acids.
- Writing research articles.
- Development of computational protocols

Requirements:

- PhD in chemistry, physics or a related discipline, with specific focus on computational chemistry, physical chemistry or molecular physics
- Expertise in using linux-based platforms (including bash) and computing servers with queuing systems.
- Prior experience with machine learning approaches in chemistry.
- Good understanding of quantum chemical methods and expertise in using quantum chemical programs such as Gaussian 16 and Orca.
- Very good knowledge of spoken and written scientific English (B2 or higher).
- Experience in writing research articles for peer-reviewed journals.
- Knowledge of programming/scripting languages such as python will be considered as an additional asset.

We offer:

- stable employment at the prestigious University,
- possibilities of career development,
- work in a creative and vibrant research team.
- additional funding for a personal computer and research related travels including collaborations and conferences.

Development prospects:

- Scientific development – University offers its employees the possibility to participate in various scientific projects and activities to improve their skills and gain experience in their chosen fields, including cooperation with other research centres and business partners.
- Education – Wrocław University of Science and Technology offers the employees the possibility to teach students and participate in dedicated training programmes.
- International cooperation – Wrocław University of Science and Technology participates in a number of programs focused on the international exchange of the Staff.

Required documents:

1. Application for entering the competition addressed to the Rector.
2. Curriculum vitae.
3. Questionnaire for the person applying for employment.
4. A copy of the document confirming obtaining the academic degree or a copy of the diploma of graduation.
5. Self-report containing information about achievements in the field of research activity, teaching experience and organizational activity.
6. List of publications.
7. List and description of scientific internships.
8. Statement on having read the information regarding the processing of personal data
9. Statement on meeting the requirements set out in Art. 113 of the Act of July 20, 2018. Law on higher education and science
10. Declaration of the candidate that in the case of winning the competition, Wrocław University of Science and Technology will be the primary place of employment*

*If a competition is won by a person who is employed under an employment relationship with another employer conducting the following activities: research, research and teaching, research and development, implementation (except for cases specified in Article 125(3) of the Act), and the employment is not expired by the date of employment at the Wrocław University of Science and Technology as the primary place of work, this person, in accordance with art. 125 sec. 1 of the Act, taking into account art. 125 sec. 2 of the Act, is obliged to obtain the Rector's consent for additional employment under an employment relationship with another employer after employing at Wrocław University of Science and Technology. If the competition is won by a person who conducts business activity, the requirement of art. 125 sec. 7 of the Act should be met.

Application documents in Polish or English should be sent:

- by e-mail to the following e-mail address rafal.szabla@pwr.edu.pl by 02.02.2024, **until 3.00 pm**

In the title of the message, please indicate the reference number: AD2/W3/01/2024

Applications of persons sending their documents without indicating a specific reference number and sent after the deadline for submission will not be considered.

All information on the course of the competition is provided by the assistant/HR assistant at the e-mail address rafal.szabla@pwr.edu.pl.

The date of receipt of the documents is decisive. The date of receipt of application documents is considered to be 3.00 pm on the day indicated in the information about the competition. Receipt of the documents from the candidate will be confirmed by the assistant/HR assistant via e-mail to the address indicated in the application.

Candidates' applications will be evaluated by the Competition Committee appointed Dean of the Faculty of Chemistry, WUST. After the competition procedure is closed, the applications of persons who have not been accepted for work will be returned, provided that they were sent by traditional mail. People interested in having their documents back will be able to pick them up from the assistant/HR assistant within 6 months after the competition procedure is closed, against acknowledgment of receipt.

LINK ENG:

https://pwr.edu.pl/fcp/gGBUKOQtTKIQhbx08SlkTUhZeUTgtCgg9ACFDC0RBSnVBG1gnBVc0FW8SETZKHg/1/public/2023/docs/zw_3_2023_zw18_-z1_eng.pdf

1) The post-doc position is awarded in accordance with the annex to the resolution of the NCN Council No. 12/2021 of March 5, 2021 amending the Regulations for granting funds for the implementation of tasks financed by the National Science Center in the field of research projects, https://www.ncn.gov.pl/sites/default/files/pliki/uchwaly-rady/2021/uchwala12_2021-zal1.pdf 2) The person to be employed in this NCN post-doc position will meet all of the following conditions:

- a) obtained a doctoral degree in 2016 or later
- b) will be selected in an open competition conducted by a recruitment committee appointed by the head of the entity implementing the research project, composed of the project manager as chairman and at least two persons indicated by him with appropriate scientific or professional qualifications. Candidates are assessed on the basis of the criteria presented in the competition announcement, and the competition results are made public by being posted on the website of the entity where the research project will be implemented;
- c) the project manager was not the supervisor or auxiliary supervisor of her doctoral dissertation;

- d) obtained a doctoral degree in an entity other than the entity where employment in this position is planned or completed at least 10-month, continuous and documented postdoctoral internship in an entity other than the entity implementing the project and in a country other than the country of obtaining the doctoral degree;
- e) will be employed for a period of not less than 6 months;
- f) during the period of receiving full-time remuneration, will not receive any other remuneration from funds allocated as direct costs from research projects financed under NCN calls;
- g) during the period of receiving full-time remuneration, he will not receive remuneration from another employer under an employment contract, including from an employer based outside Poland.

The University stipulates that the competition may not be concluded.

Public documents:

The consolidated text of the Regulations for conducting open competitions for the position of an academic teacher and other necessary documents can be found here:

LINK PL, EN: <https://wch.pwr.edu.pl/pracownicy/konkursy>

Recruitments and competitions conducted by Wrocław University of Science and Technology are open, carried out in accordance with clear and transparent rules based on clear and unambiguous criteria of substantive evaluation, taking into account a diverse professional career. Wrocław University of Science and Technology conducts recruitment procedures in accordance with the guidelines of the European Charter for Researchers and the Code of Conduct for the Recruitment of Researchers and the Open, Transparent and Merit-based Recruitment Policy (OTM-R) at Wrocław University of Science and Technology.

Recruitments and competitions conducted by Wrocław University of Technology and Science are conducted taking into account the policy of equal opportunities in accordance with the "Equality plan for Wrocław University of Science and Technology for the period 2022–2024"

LINK PL: <https://rowna.pwr.edu.pl/aktualnosci/plan-rownosci-dla-pwr-11.html>

LINK EN: <https://rowna.pwr.edu.pl/en/>