



UNIVERSITY
OF WARSAW

Faculty of Chemistry



WCH.1210-16/2022

Post Doc Position in a NCN SONATA project:
**Dynamic Quantum Crystallography for accurate structures,
entropy and other thermodynamic properties for molecular
crystals**

Overview

The objective of the project is the development of a new methodological approach for X-ray data refinement with the goal of evaluation of molecular crystal thermodynamic properties that take into account vibrational and configurational entropy contributions to free energies of molecular crystals based on the combination of accurate *ab-initio* calculations and statistical methods. Obtaining thermodynamic properties from X-ray diffraction data and calculations would be a significant breakthrough - understanding stability of a molecular solid state is still one of the hottest topics in crystallography, chemistry, pharmacy and physics.

We seek to recruit a self-driven and creative theoretical chemist to join our team to work on NCN SONATA project entitled "Dynamic Quantum Crystallography for accurate structures, entropy and other thermodynamic properties for molecular crystals".

The post-doc (adiunkt w grupie pracowników badawczych) will run a research in exact and natural sciences, in discipline of Chemical Sciences. Available positions: 1.

Responsibilities include:

- conducting theoretical calculations (mostly DFT for periodic systems)
- keeping scientific documentation;
- creating publications from research results;
- sharing of knowledge with PhD students and undergraduates in theoretical research.

Qualifications

- PhD in Crystallography, Computational Chemistry or related field

Required:

- Good knowledge of DFT calculations;
- Good knowledge of single crystal X-ray diffraction principles;
- Self-driven, proactive, and forward-thinking attitude.

Considered a plus:

- Programming.

Personal attributes

- Highly organized, conscientious, and reliable team player, with strong attention to detail;
- Excellent communication and presentation skills to share complex ideas and results with non-experts;
- Fluency in English.

The candidate must meet the requirements of art. 113 of the Act - Law on Higher Education and Science dated July 20, 2018 (Journal of Laws of 2021, item 478).

Your benefits

- The total salary before taxing (brutto/brutto) is 10 000 PLN/month;
- Ample support to grow your skills;
- Contract with the University of Warsaw (full time position/employment contract at Faculty of Chemistry for a 2 years with possibility of extension, at assistant professor in group of science position)

Please send your

- CV,
- motivation letter,
- publication record,
- information on the processing of personal data (the template available at: <http://www.chem.uw.edu.pl/oferty-pracy/>),
- declaration of reading and acceptance of the rules for conducting competitions at the University of Warsaw (a template available at: <http://www.chem.uw.edu.pl/oferty-pracy/>,
- references

no later than **5th of October 2023** to a.hoser@uw.edu.pl adding "Post Doc position" to the subject of your email.

The results of the competition will be given by e-mail till October 16th, 2023.

The competition is the first stage of the employment procedure as an academic teacher, and its positive outcome is the basis for further proceedings.