

## Post Doc Position

### Dynamic Quantum Crystallography for accurate structures, entropy and other thermodynamic properties for molecular crystals

## Faculty of Chemistry, University of Warsaw Warsaw, Poland

### 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 SONATA project entitled “Dynamic Quantum Crystallography for accurate structures, entropy and other thermodynamic properties for molecular crystals”.

### Responsibilities include

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

### Qualifications

- PhD in Crystallography, Computational Chemistry or related field - hold at the first day of the contract (applications from PhD students are accepted)

### 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 2018, item 1668 as amended).

## **Your benefits**

- The total salary before taxing (brutto/brutto) is 10 000PLN/month;
- Ample support to grow your skills;
- Contract with the University of Warsaw (full time position/employment contract)

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 **25<sup>th</sup> of September** to [a.hoser@uw.edu.pl](mailto: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 1st, 2022. Only candidates who submit complete documentation will be considered in the recruitment procedure. In the case of not signing the contract by the candidate, due to the resignation, we reserve the right to choose the next candidate from the ranking list. The competition may be repeated until a suitable candidate who fulfils all requirements is found.