



UNIWERSYTET  
WARSZAWSKI

Wydział Chemii



WCH.1210-17/2019-1

Warsaw, 9.03.2020

## An announcement for **adjunct (postdoc)** position

High paying position for **adjunct (post doc)** who will develop new models and software in a project at borderline of crystallography and computational chemistry entitled "**Advancing quantum crystallography for better insight into structure and properties of crystals**" financed by **National Science Centre (NCN)** is open for application.

Project leader: **Prof. dr hab. Krzysztof Woźniak**

Grant Decision: **NR DEC-2018/31/B/ST4/02142**

Available positions: 1 (a group of researchers operating in the field of exact and natural sciences).

### **We are looking for a motivated candidate:**

1. **Adjunct (postdoc)** who will be responsible for progress in programming and creation of the software and model related to Hirshfeld Atom Refinement (HAR) method.

### **We expect a person with:**

- a PhD degree in chemistry or physics, informatics, mathematics or related fields,
- experience in programming, preferred C++ and/or Python.
- experience in a research involving computational modeling combined with development of related software/code is preferred
- knowledge of crystallography, solid state physics, computational chemistry and numerical methods is an advantage
- excellent analytical and problem-solving skills
- ability to work independently and within a team

### **The ideal candidate would also have:**

- experience in ab-initio computational chemistry methods including those for large molecules
- experience in quantum crystallography
- experience in crystallographic refinement (especially in HAR)
- familiarity with charge density related calculations

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).

**We offer:**

- A temporary contract with the University of Warsaw (full time position/employment contract) since 1st June 2020 till 30th September 2022.
- Work in friendly environment in a rapidly developing research field.
- The total salary before taxing is 15 000 PLN/month (~10 000 PLN net ≈ 2350€).
- The opportunity to present results during scientific conferences and in well-recognized scientific journals.

**The project:**

aims at creation and validation of new methods of extraction of more accurate and precise structural information (geometrical, electronic and thermal parameters) from single crystal X-ray diffraction (XRD) experiments than this is possible by using presently available methods of refinement of X-ray data. This will be achieved by advancing quantum crystallography methods (in particular extensions of Hirshfeld Atom Refinement – HAR) well beyond the present state-of-the-art. The current implementation of HAR is, in practice, limited to a certain class of small molecules because for larger molecules computation are by far too long. Our application aims at a significant extension of capabilities of the HAR approach to cover broader range of systems which can be in practice investigated with the method as well as drastically speed up related calculations.

**Required documents:**

- Motivation letter
- Curriculum Vitae (CV),
- Information on the processing of personal data and declaration of the acceptance of the competition rules at the University of Warsaw (the templates available at: <http://www.chem.uw.edu.pl/oferty-pracy/>),
- List of publication (and/or pieces of software created) highlighting the three most important works
- short description of the 3 most important achievements
- 1 confidential opinion of the promoter (or a researcher) who supervised your research work sent directly to the e-mail address: qc@chem.uw.edu.pl

Please submit the documents **no later than 10<sup>th</sup> April 2020** to: **qc@chem.uw.edu.pl** (PDF is the preferred format). E-mail entitled: “**QC Adjunct 1**”

Selected candidates will be informed about the date of the interview by e-mail until **15<sup>th</sup> April 2020**. The results of the competition will be given by e-mail till **20<sup>th</sup> April 2020**. In justified cases, the interview may also take place via the Internet. Only those who submit complete documentation will be considered in the recruitment procedure.

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