UNIWERSYTET WARSZAWSKI
Wydział Chemii

Warsaw, 7.08.2019.

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An announcement for adjunct position

Position of **adjunct (group of research workers)** in the project 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.

We are looking for motivated candidate:
Adjunct (programmer) who will be responsible for progress in programming and creation of the software related to Hirshfeld Atom Refinement method.

We expect a person with:

- a PhD degree in chemistry or physics, informatics, mathematics or related fields,
- experience in programming, strongly preferred C++ and/or Python.
- experience in computational quantum chemistry and/or crystallography fearlessly face other people's code,
- knowledge of crystallography, solid state physics, computational chemistry,
- experience in initiation, performing and reporting interdisciplinary studies,
- excellent oral and written knowledge of English,
- ability to work independently and within a team,
- excellent analytical and problem-solving skills,
- excellent debugging and critical thinking skills,
- analytical skills and practical knowledge of writing scientific texts.

Additional skill and abilities expected:

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

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 Faculty of Chemistry University of Warsaw (full time position/employment contract) from **2/10/2019 to 30/09/2022.**

Required documents:

- Motivation letter

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- Curriculum Vitae (CV),
- information on the processing of personal data (use a template available at website: 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 20/08/2019** 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 **30/08/2019**. The results of the competition will be given by e-mail till **15/09/2019r**.
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 total salary before taxing (brutto/brutto) is 15 000PLN/month.

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

Abstract of the project: „Advancing quantum crystallography for better insight into structure and properties of crystals".

Research project objectives/Research hypothesis. This 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 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 large molecules with the help of quantum chemical methods especially designed for such systems (significantly reducing computing time) and disordered structures so common in crystallographic studies.

As the stockholder(Hirshfeld) method of partitioning of electron density into atomic contributions, which is used in HAR, can been extended and there exist more approaches rooted in this partitioning and showing certain advantages over the original method, we plan to test the alternative approaches in HAR like refinement and compare their performance to the original HAR method and other classical methods of refinement.

We also plan to create a databank of a Hirshfeld atomic electron densities derived directly from quantum chemical calculations. Such ready bricks of electron density can be used to reconstruct electron density in proteins, and small molecules, and they should preserve some advantages of the quantum chemical model of electron density at drastically reduced computational costs of refinement particularly in the case of macromolecules.

Research project methodology. Realization of the proposed advancements requires:

- development of a new software platform for testing novel approaches for crystal structure refinement. This would involve basic and flexible refinement program as well as tools for integration of the new developments with mature commonly used crystallographic refinement codes. Availability of this kind of tools is essential for rapid testing of new ideas and methodologies.

-verification of the true precision and accuracy of the proposed new methods by statistical analysis of results of multiple X-ray measurements and refinements of the collected data performed for a series of model crystals of increasing complexity to prove broad applicability of new solutions. Our results will be compared to the precision and accuracy of IAM structural results (+multipolar refinement and original HAR methods). The series consists of single crystals of the following compounds: a few simple model organic compounds such as, for example, oxalic acid, glycine, carboxylic acid salts and complexes, more complex metalorganic compounds with different metal ions and hydrogen atoms and small and larger proteins such as lysozyme, crambin etc. As original HAR seems to work correctly even for small resolution, we also want to test its applicability in high pressure structural studies.

Expected impact of the research project on the development of science. Proposed enhancements are intended to effectively replace a 100-years old and too much simplified, spherical Independent Atom Model (IAM) of atomic electron density in the refinement of structural/electronic models of crystals against intensities of scattered X-ray beams (these are ca. 99.7% of all refinements performed so far for ca. 1.4mln of crystal structures) and to replace more modern methods of refinement based on aspherical scattering factors such as multipole refinement or refinements based on databanks of pseudatoms or original HAR (ca. 0.3% of all refinements). By improving HAR we will improve quality of structural information extracted from measured intensities of X-ray reflections. This will help in solutions or different structural and electronic problems in different fields of science particularly on the biol/chem/phys interface.

Pioneering nature of the research project. Recent introduction of Hirshfeld Atom Refinement (HAR) has already led to a paradigm shift in the precise determination of hydrogen atom positions now possible with HAR against single crystal X-ray data. HAR is an excellent example of Quantum Crystallography (QC) - a new emerging field of science that aims at extracting information from different experiments (including X-ray experiments) by adopting a quantum mechanical approaches. Advancing HAR beyond the present state-of-the-art means broadening borders of modern crystallography and through a better quality of structural information creating new chances for solving problems in other fields of science such as medicine, pharmacy, materials science, physics, biology, chemistry, etc.