



UNIWERSYTET
WARSZAWSKI

Wydział Chemii



WCH.1210-2/2020-1

18/02/2020, Warsaw (Poland)

An announcement for adjunct position

Position of **adjunct (group of research workers)** in the project entitled "**Phase transitions in minerals induced by pressure and studied by experimental charge densities - feasibility studies**" financed by **National Science Centre (NCN)** is open for application.

(see: <https://crystal.chem.uw.edu.pl/>)

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

Grant Decision: **NR DEC-2019/33/ B/ST10/02671**

Available positions: 1 post-doc operating in the field of exact and natural sciences.

We are looking for a highly motivated candidate: Adjunct (advanced crystallographer) who will be responsible for: collection of X-ray data at ambient conditions and under pressure, data analysis and refinement of structures, refinement of experimental electron densities for minerals, analysis of details of electron densities, complementary theoretical calculations for periodic systems and clusters of molecules, programming some fragments of code needed for data analysis, supervision of PhD students and undergraduate students

We expect a person with:

- PhD degree (or equivalent degree) in crystallography, mineralogy, chemistry or physics, informatics, or related fields obtained within last 6-7 years,
- postdoctoral experience in experimental charge density investigations and/or high pressure studies of crystals,
- experience in applications of computational quantum chemistry to periodic systems,
- knowledge of crystallography, mineralogy, solid state physics, inorganic crystal structures, studies of crystal under high pressure,
- experience in initiation, performing and reporting interdisciplinary studies
- excellent knowledge of written and spoken English, written and spoken presentation skills
- ability to work independently and within a team
- excellent analytical and problem-solving skills
- practical knowledge of writing scientific texts

Additional skills and abilities expected :

- experience in quantum crystallography
- experience in ab-initio computational chemistry methods including those for periodic systems

We offer:

a temporary contract with the University of Warsaw (full time position/employment contract) from **1.05.2020 to 31.03.2023**.

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 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: mincryst@chem.uw.edu.pl

Please submit the documents **no later than 19.03.2020** to:

mincryst@chem.uw.edu.pl (PDF is the preferred format). E-mail entitled: **"MinCryst Adjunct 1"**

Selected candidates will be informed about the date of the interview by e-mail until **23.03.2020**. The results of the competition will be given by e-mail till **16.04.2020r**. In justified cases, the interview may also take place *via* internet. Only those who submit complete documentation will be considered in the recruitment procedure. Up to the best 6 candidates will be invited for interviews.

The total salary before taxing (brutto/brutto) is 10 000PLN/month

Abstract of the project: " Phase transitions in minerals induced by pressure and studied by experimental charge densities - feasibility studies".

Mineralogy and crystallography have common roots. For centuries the main subject of crystallographic studies were minerals. Only at the beginning of the twentieth century did these two branches of science separate. Crystallography focused mainly on the development of new research methods (including those based on X-ray diffraction), while mineralogy focused on the properties of minerals. Both these branches of science are combined in X-ray studies of the structure and properties of minerals. Almost all (ca. 99.7%) out of 1.5mln known crystal structures have been determined by applying a 100-year old spherical Independent Atom Model (IAM) in the refinement of X-ray data. This also includes almost all minerals (ca. 5500). IAM was proposed by W. H. Bragg in 1914. It is a great paradox that researchers use now sophisticated synchrotrons and diffractometer and then refine more than a century old model (IAM) of electron density in crystals/minerals.

There are only a few thousands of crystal structures refined by aspherical approaches such as quantitative Multipole Refinement (MR) of electron density or Hirshfeld Atom Refinement (HAR). This includes ca. 35 minerals refined within last 50 years by multipole refinement including published by us electron density of fluorite. We have just refined experimental electron density for single crystal of grossular under pressure **and up to our knowledge this is the very first successful refinement of quantitative electron density in minerals under pressure using multipole refinement**. These results and a new design of Diamond Anvil Cell with wider opening angle (up to 120° allowing for up to 50GPa pressure) opens completely new field of mineralogical studies.

So the aim of this project is to apply MR in pioneering combination of experimental charge densities with high pressure and variable temperature studies of minerals and processes they undergo. We plan to perform feasibility studies of phase transitions in model minerals induced either by applying

pressure or temperature (or both stimuli). We want to select minerals which undergo phase transitions below 50GPa, diffract well enough at high diffraction angles (this is a must for experimental charge densities), and for which - at least for some of them – phase transitions have already been studied at the structural level by using routine methods. **We will practically demonstrate how far deeper insight can be gained by applying multipole refinement of experimental electron densities in minerals comparing to routine structural studies.** This includes the following: -far better (more precise and more accurate) geometrical (bond lengths and valence angles) and thermal (ADPs) parameters of atoms in minerals; - possibility of tracing flow of charge (charge transfer) among ions in the crystal lattices of minerals under variable pressure or temperature, reliable experimental topology of charge distributions and charge and volumes of ions forming crystal lattices of different phases of minerals – this will allow for more reliable theoretical modelling of ionic crystals - and point and integrated electron density parameters at critical points of electron density distributions and at other key points of the mineral structures studied (for example deviations from sphericity of ions in crystal lattices of minerals); -reliable estimates of energy of electrostatic interactions, electrostatic potential (ESP) and its parameters in minerals, electric field gradient and, in general, all one electron properties of atom which can be correlated with different mineralogical and physicochemical properties of minerals; -we also want to explain the nature of changes of the most important interactions which determine phase transitions particularly at the level of changes of details of electron density and analyse the most important factors influencing phase transitions).

The phase transitions in the following minerals will be studied (of course only when different phases of these minerals diffract well enough at high diffraction angles): **Kyanite** [from Brazil and from the Kola Peninsula, Russia, Al_2SiO_5 , Triclinic, P-1], **Diopside** [Bazenowskoje, Russia, $\text{CaMgSi}_2\text{O}_6$, Monoclinic, C2/c], **Enstatite** [Kraubath, Austria, $\text{Mg}_2\text{Si}_2\text{O}_6$, Orthorhombic, Pbc], **Pyrope** [Czechia and Italian Alps, $\text{Mg}_3\text{Al}_2(\text{SiO}_4)_3$, Cubic, Ia3d], **Olivin, Forsterite** [from Vesuvius volcano and Norway Mg_2SiO_4], **Wollastonite** [(from Garby Izerskie, Poland, $\text{Ca}_3\text{Si}_3\text{O}_9$ Triclinic, P-1], **Brucite** [from N'chwanging II Mine, RSA, $\text{Mg}(\text{OH})_2$, Trigonal, P-3m], **Quartz** (α and β) [SiO_2], **Boracite** [$\text{Mg}_3\text{B}_7\text{O}_{13}\text{Cl}$, Orthorhombic, Pca2₁], **Diamond** and **Graphite** and other interesting minerals and new phases undergoing phase transitions.

This project is important for purely scientific reasons related to understanding the nature of phenomena occurring in minerals but also important for geophysicists describing methods of propagating seismic waves in the Earth's mantle and those dealing with various models of gravitational phenomena, mineralogists involved in modeling distribution of admixture of trace elements in minerals and ways to redistribute them during phase changes. Over 100 years after the Bragg research, we offer new possibilities in mineralogical research