



UNIWERSYTET
WARSZAWSKI

Wydział Chemii



WCH.1210-...../2019

Warszawa (Poland) 30/07/2019

Job offer for a PhD student position

Position of **PhD student** in the project entitled „**Modelling of crystal and magnetic local structure in potential quantum spin liquid (QSL) alpha-RuCl₃**” financed by **National Science Centre (NCN)** is open for application.

Project leader: **dr Wojciech Sławiński**

Grant Decision: **NR DEC-2018/31/B/ST4/00943**

Available positions: 1.

We expect a person with:

- MSc degree in chemistry, physics or related field,
- practical knowledge of advanced crystallography methods at the MSc level (confirmed by publications if possible) including knowledge of symmetry, X-ray structural analysis).
- experience in crystal structure analysis by using diffraction methods (single and monocrystalline materials) using laboratory X-Ray sources, synchrotron radiation and/or neutrons.
- experience in performing crystallographic measurements
- experience in crystallization
- excellent oral and written knowledge of English
- ability to work within a team

Additional skills and abilities expected:

- programming in Fortran, C++ and/or Python
- experience in using Linux/Unix

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).

We offer:

PhD stipend at the University of Warsaw from **1/10/2019 to 30/09/2022**.

Required documents:

- Motivation letter
- Curriculum Vitae (CV),
- information on the processing of personal data (see the text below),
- List of publication (and/or pieces of software created) highlighting the three most important works

- short description of the 2 most important achievements
- 1 confidential opinion of the promoter (or a researcher) who supervised your research work sent directly to the e-mail address:
wslawinski@chem.uw.edu.pl

Please submit the documents **no later than 20/09/2019** to:
wslawinski@chem.uw.edu.pl (PDF is the preferred format). E-mail entitled: „**RuCl3 PhD student**”

Selected candidates will be informed about the date of the interview by e-mail until **23/09/2019**. The results of the competition will be given by e-mail till **25/09/2019r**. 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 stipend is 4 500 PLN / month (nontaxable)

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

INFORMATION ON THE PROCESSING OF PERSONAL DATA

INFORMATION CLAUSE

Pursuant to Article 13 of Regulation (EU) 2016/679 of the European Parliament and of the Council of 27 April 2016 on the protection of natural persons with regard to the processing of personal data and on the free movement of such data, and repealing Directive 95/46/EC (General Data Protection Regulation), University of Warsaw hereby informs:

1. The Controller of your personal data is the University of Warsaw with its registered office at Krakowskie Przedmieście 26/28, 00-927 Warszawa;
2. The Controller has designated the Data Protection Officer who supervises the processing of personal data, and who can be contacted via the following e-mail address: iod@adm.uw.edu.pl;
3. Your personal data will be processed for the purpose of carrying out a recruitment process and selecting an employee and concluding a contract for employment at the University of Warsaw;
4. The provided data will be processed pursuant to Article 22¹ § 1 of the Act of 26 June 1974 Labor Code (uniformed text: Dz.U. of 2018, item 917) and your consent for processing of personal data;
5. Provision of data in the scope stipulated in the Labor Code is mandatory, and the remaining data are processed according to your consent for processing of personal data;
6. The data will not be shared with any external entities;
7. The data will be stored until you withdraw your consent for processing of personal data;

8. You have the right to access your personal data, to rectify, erase them, restrict their processing, object to processing, and to withdraw the consent at any time;
9. You have the right to lodge a complaint to the President of the Office for the Protection of Personal Data.

CONSENT CLAUSE

I hereby consent to have my personal data processed by the University of Warsaw with its registered office at Krakowskie Przedmieście 26/28, 00-927 Warszawa for the purpose of carrying out a recruitment process and selecting an employee and concluding a contract for employment at the University of Warsaw.

I have been informed of my rights and duties. I understand that provision of my personal data is voluntary.

.....
.....

(place and date)

(signature of the person applying for employment)

Abstract of the project: „Modelling of crystal and magnetic local structure in potential quantum spin liquid (QSL) α - RuCl_3 ”

The coupling of properties of materials with their crystal structure is currently one of the main topic of modern crystallography. Finding connections between material's crystal structure, local order and its local distortion and the average structure with chemical and physical properties of the materials is within the scope of interest of many research groups worldwide. One of the intensively studied research areas in the field of magnetic materials is to seek for candidates for Quantum Spin Liquid (QSL) state.

QSL is an exotic state of matter where in the ground state, strongly coupled magnetic moments do not show any long range ordering even down to the lowest temperature around 0K. The ground state is a superposition of many, fluctuating states, of different magnetic moment orientations [1]. As a consequence, it is predicted in QSL state to find quasiparticles called Majorana fermions as excited states [2]. The group of materials where potentially QSL state can be found is honeycomb type lattice. It is possible within this class of materials to realize the QSL state by atoms which carry $\frac{1}{2}$ spin. The physical model describing this class of materials is called the Kitaev model [3]. The existence of SQL state in the Kitaev type structures has not yet been experimentally proven. This problem is now intensively studied to find examples of such materials. One of the QSL examples is a molecular crystal κ -(BEDT-TTF) $_2\text{Cu}_2(\text{CN})_3$, where no long range magnetic moment ordering has been observed even down to 20 mK [4].

One of the group of materials with possible QSL states, are those materials with the layered structure, where atoms with magnetic moment (spin of $\frac{1}{2}$) are located

in two dimensional slabs. Those layers are later arranged into three dimensional structure one layer on top of the other one (in fact the layers are complemented in such a way that the atoms from one layer are closing voids in the other one). An example of such a compound is α -RuCl₃, where 2D layers forms 3D structure by weak Van der Waals interactions. This is why it is highly probable to observe faults in the 3D arrangement of 2D layers in those crystals. This means that it is likely to observe deviations from the 3D periodic close packing. Those defects are called “stacking faults” and are an intrinsic structural property of a given material. In the case of stacking faulted structure, the 3D translational symmetry is not conserved in the direction perpendicular to the 2D crystalline layers.

There are many models of the QSL type phenomenon. The main reason of that variety is that the structure of those materials is likely to be of the stacking fault type. Within the scope of the project, it is planned to investigate crystal structure of α -RuCl₃ as a function of temperature. The obtained model will be possible to be used in further studies and magnetic calculations. Since the structure has layered nature, it will be required to use tools dedicated to modelling of stacking faulted materials.

The second part of the project is to study the local disorder in those materials. The Bragg diffraction delivers precise information about the average structure of these materials. In the case of partially disordered materials, it is likely that the local positions of atoms show significant distortions from the average crystal structure. This can have a significant impact especially on magnetic interatomic interactions. Local disorder or local short range order can be studied by one of the powder diffraction method called Pair Distribution Function (PDF). Also the short range order of magnetic moments can be studied by this diffraction method. This will require further development of the RMCProfile program [5]. The measurements and data analysis of PDF will allow for describing local crystal structure and its correlation with the magnetic ordering.

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[2] Kitaev, A. *Ann. Phys.* 321, 2016, 2

[3] R. D. Johnson, S. C. Williams, A.A. Haghighirad, J. Singleton, V. Zapf, P. Manuel, I. I. Mazin, Y. Li, H. O. Jeschke,

R. Valenti, and R. Coldea, *Phys Rev. B* 92, 235119 (2015)

[4] P. Lampen-Kelley, A. Banerjee, A.A. Aczel, H.B. Cao, M.B. Stone, C.A. Bridges, J.-Q. Yan, S.E. Nagler, and D.

Mandrus, *Phys. Rev. Lett.* 119, 2017, 237203

[5] M. G. Tucker, D. A. Keen, M. T. Dove, A. L. Goodwin and Q. Hui, *J. of Phys. Cond. Mat.* 19, 2007, 335218