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Wydział Chemii



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### An announcement for adjunct position

Position of **adjunct (group of research staff)** in the project entitled „**Modelling of crystal and magnetic local structure in potential quantum spin liquid (QSL) alpha-RuCl<sub>3</sub>**” 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:

- PhD degree in chemistry, physics or related field (obtained after 1/10/2012 according to NCN rules ([www.ncn.gov.pl](http://www.ncn.gov.pl))),
- experience in programming (preferred Fortran, C++ and/or Python),
- ability of analysis/using computer code written by others,
- knowledge of crystallography, solid state physics,
- experience in experimental diffraction methods (single and polycrystalline samples) by using standard methods
- experience in analysis of experimental diffraction data by Pair Distribution Function method
- excellent oral and written knowledge of English, proven by writing scientific texts
- experience in conducting diffraction experiments
- ability to work independently and within a team
- excellent analytical and problem-solving skills
- excellent debugging and critical thinking skills

Additional skills and abilities expected:

- knowledge of Linux/Unix operating system
- experience in code optimization in programming
- experience in crystallization

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) from **1/01/2020 to 31/12/2021** with possibility of extension.

#### Required documents:

- Motivation letter
- Curriculum Vitae (CV),
- information on the processing of personal data (the template 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: wslawinski@chem.uw.edu.pl

Please submit the documents **no later than 10.11.2019** to: **wslawinski@chem.uw.edu.pl** (PDF is the preferred format). E-mail entitled: **“RuCl3 PostDoc”**

Selected candidates will be informed about the date of the interview by e-mail until **20/11/2019**. The results of the competition will be given by e-mail till **12/12/2019**. 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 10 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: „Modelling of crystal and magnetic local structure in potential quantum spin liquid (QSL) $\alpha$ - $\text{RuCl}_3$ ”

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  $\kappa$ -(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  $\alpha$ - $\text{RuCl}_3$ , 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  $\alpha$ - $\text{RuCl}_3$  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.

[1] L. Balents, Nature 464, 2010, 199

[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. Let. 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