

# Graduate Student Positions in Winnipeg, MB, Canada

We are looking for three or more qualified graduate students (M.Sc. or Ph.D. level) to join the Schreckenbach and Hollett research groups.

## Background:

An applicant must have – or be close to receiving – a B.Sc., M.Sc. or equivalent in chemistry or physics or a closely related field. A good knowledge of, and a strong interest in, physical chemistry, computational chemistry and/ or inorganic and materials chemistry are essential. Proof of English language proficiency is required. Programming experience is important for some of the projects.

## Research projects (Schreckenbach research group):

The following projects are of particular interest.

- (1) “*Program development within the ADF and ADF-BAND environments*”. Programming experience is required for this project. Knowledge of quantum-chemistry codes such as ADF, ADF-BAND, and band-structure codes *etc.* are assets. For this project, students with a degree in physics and relevant experience and background (e.g. in band-structure methods) are also encouraged to apply.
- (2) “*Theoretical actinide molecular science*”. This area is a long-standing interest of my group. The specific project will be defined at a later stage, but it may involve modeling metal-protein interactions or organometallic actinide chemistry, the latter based on various collaborations with experimental groups.
- (3) “*2D materials*”. A variety of 2-dimensional materials will be modeled. Potential projects include studying the influence of chemical modifications and interfaces with polymers.

In addition to these two areas, the following topics are of interest as well.

- (4) “*Environmental mercury chemistry*”. Computational study of mercury complexes, with a focus on environmental chemistry. Future directions might include gas-phase (atmospheric) chemistry or dynamics studies of mercury solvation.
- (5) “*Polymer modeling*”. Modeling of conducting polymers, with a view of applications in novel memory devices or solar energy conversion.
- (6) “*Solar energy*”. We are using the tools of computational quantum chemistry to understand elementary chemical processes within dye-sensitized solar cells (DSSC) and to study singlet-fission materials.
- (7) *Other projects as initiated by the student are possible in principle.*

These specific projects are embedded into the general research program of my group. (See my homepage for further details.)

## Research projects (Hollett research group):

Positions are currently available for students interested in the development of quantum chemistry tools for the study of complex chemical problems. Experience with programming and scripting languages is not required but certainly an asset.

- (1) “*New approaches to the correlation problem*”. We have recently devised our own approach, the  $\Delta$ NO-method, to modeling electronic structure. Current efforts involve testing against thermochemical and kinetic data test sets, improving efficiency of optimization algorithms, implementation of nuclear gradients, and the incorporation of 'linear-scaling' methodology.
- (2) “*The  $\Delta$ NO-method for excited states*”. We are currently exploring the treatment of excited states using our newly developed method.

(3) “*New correlated methods for materials*”. We are extending a modified version of our  $\Delta$ NO-method to periodic (2D and 3D) systems to develop a (relatively) low cost approach to modeling the correlated electronic structure of materials.

**Application:**

Interested candidates should contact Dr. Schreckenbach directly by E-mail, and provide *all of the following material*:

- Cover letter;
- A detailed CV including list of publications (if any);
- Detailed lists of courses and grades or preferably scanned (unofficial) copies of transcripts;
- Names and E-mail addresses of two or more potential referees;
- Document outlining in detail which of the project(s) are of particular interest to you and why (approximately 1–2 pages).

In addition, please provide the following information in your CV, cover letter or in separate documents:

- Comment on your English proficiency (e.g. TOEFL, IELTS, or native speaker);
- Comment specifically on your background in relevant areas such as quantum mechanics, programming, inorganic chemistry, materials chemistry, physics, mathematics;
- Please mention where you found this advertisement;
- Comment on the preferred start date. Potential start dates are Sept. 1, 2017, Jan. 1, 2018 or May 1, 2018. Non-Canadian applicants should keep in mind that visa processes take considerable time. (This would make the September start date unlikely.)

**Application process:**

The review of the applications will begin on May 15, 2017 and will continue until the positions are filled. We expect to create a shortlist by the end of June. At this point, shortlisted candidates will be invited to submit a formal application. Admission into our graduate program is the *joint responsibility* of the Department of Chemistry and the Faculty of Graduate Studies at the University of Manitoba, see: [http://www.umanitoba.ca/faculties/graduate\\_studies/](http://www.umanitoba.ca/faculties/graduate_studies/)

After successful admission, candidates will receive an official admission letter that will allow them to apply for Canadian visa if required.

**Schreckenbach research group:**

The research of my group is focused on developing density functional theory (DFT) based methods and applying them to study molecules and their properties. For more details, please contact me directly or refer to my web pages at: <http://home.cc.umanitoba.ca/~schrecke/>

**Hollett research group:**

More on our group (interests, members, publications) can be found at: <http://ion.uwinnipeg.ca/~jhollett/hollettgroup.html>

**Environment:**

The Schreckenbach research group is part of the Department of Chemistry at the University of Manitoba in Winnipeg. The University of Manitoba (<http://www.umanitoba.ca/>) is the largest university in the province of Manitoba and among Canada’s major research universities. It has an undergraduate student population of about 25,000, and about 4,000 graduate students. The Chemistry Department (<http://www.umanitoba.ca/chemistry/>) is one of the largest departments in the University of Manitoba, yet it keeps a friendly and collaborative atmosphere. Recently, the department has undergone a period of renewal and growth.

The Hollett research group is part of the Department of Chemistry at the University of Winnipeg (<https://www.uwinnipeg.ca/>). The University of Winnipeg is located at the centre of the city and recent additions to infrastructure, including the Richardson College for the Environment (home of the Chemistry Department), have helped it play a key role in revitalizing the downtown area.

Winnipeg (<http://www.winnipeg.ca/>) is a prairie city with a population of approximately 730,000 (metro area). Its people come from various ethnic backgrounds, and are generally friendly and welcoming. Cultural amenities include ballet, theatre, symphony, ethnic festivals, and museums, and professional sports teams are popular. Winnipeg is a safe city. It is located close to good outdoor recreational activities with a wide variety of lakes, beaches and wilderness areas within an easy drive of the city.

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