

Graduate Student Position(s) in Winnipeg, MB, Canada

I am looking for a qualified graduate student (M.Sc. or Ph.D. level) to join my research group. Depending on funding, it is possible that one or two additional positions open later this year.

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, computational chemistry and/ or inorganic chemistry are essential. Proof of English language proficiency is required. Programming experience is essential for the first project.

Research projects:

The following projects are of particular interest.

- (1) “*Program development within the ADF-BAND environment*”. Programming experience or experience with quantum-chemical program systems are required for this project. Knowledge of topics such as ADF, ADF-BAND, 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. In its current form, this project would be an M.Sc. project, although extensions to a Ph.D. are possible in principle, e.g. by combining it with one of the other areas.
- (2) “*Theoretical actinide molecular science*”. This area is a long-standing interest of my group. At the current time, we are studying (i) complexes between actinides (U, Np, Pu) and macrocycles, (ii) the interaction of aqueous actinyl species with mineral surfaces, (iii) aqueous actinide species, (iv) gas-phase reactions of actinide molecules.
- (3) “*Dye-sensitized solar cells*”. We are using the tools of computational quantum chemistry to understand elementary chemical processes within dye-sensitized solar cells (DSSC). Currently, the development of (i) high-throughput computational (HTC) tools for prescreening dyes, (ii) complex molecular models for DSSC components are of particular interest.
- (4) “*Polymer photovoltaics*”. I anticipate developing a new research project in this general area; accordingly there is considerable room for the student to influence and drive the direction of this research. Hence, for this project, a background in related areas such as polymer modeling or solar cell modeling is necessary.

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

- (5) Modeling of novel mesoscopic electronic memory devices. This is a new project that involves going from the molecular nano-scale to larger length ranges and thus coarser models.
- (6) *Environmental mercury chemistry*. Computational study of mercury complexes, with a focus on environmental chemistry. Future directions might include novel molecular sensor or dynamics studies of mercury solvation.
- (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.)

Application:

Interested candidates should contact me 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 or native speaker);
- Comment specifically on your background in relevant areas such as quantum mechanics, programming, inorganic chemistry, physics, mathematics;
- Please mention where you found this advertisement;
- Comment on the preferred start date. Potential start dates are July 1, 2014, Sept. 1, 2014 and Jan. 1, 2015. Non-Canadian applicants should keep in mind that visa processes take considerable time.

Application process:

The review of the applications will begin March 31, 2014 and will continue until the position(s) are filled. I expect to create a shortlist by the end of April. At this point, shortlisted candidates will be invited to submit a formal application. Admission into our graduate program is the *joined 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/

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

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/>

Environment:

My 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.

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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