

Job Title: Research Scientist, X-ray Crystallography

**Department:** Chemistry

Reports To: Chemistry Department Chair

Jobs Reporting: None

Salary Grade: USG 11

Effective Date: December 2022

#### **Primary Purpose**

The X-ray Crystallography Laboratory provides service to support research operations of department members as well as to provide occasional service to individuals and agencies external to the department and external to the University of Waterloo on a fee for service basis. The X-ray Research Scientist manages the day-to-day operation and maintenance of the facility which houses very valuable and sensitive scientific equipment. The role interacts and supports users (faculty, staff and students) as well as some external users from Canadian Universities and industry to assess research needs and troubleshoot technical issues. The X-ray Research Scientist is accountable to the Department Chair of Chemistry for operation, administrative and technical issues in the facility.

#### **Key Accountabilities**

# X-ray Crystallography Laboratory/Facility Support

- Maintain and safely operate X-ray equipment under the jurisdiction of the Department of Chemistry X-ray Crystallography Users committee
- Ensure the instrument performance conforms to standards required for reporting research results
- Responsible for the acquisition of X-ray crystallographic data for clients
- Instruct users of the facility on the procedures to have samples analyzed by the Research Scientist
  and facilitate their access to the facility as needed
- Undertake research projects, both independently and in collaboration with faculty members. Such
  research may be in the areas of development of new instrumentation and/or techniques
- Solve complex technical problems with the equipment which could include software, hardware or experimental set-ups
- Actively seek contracts with external users as time permits
- Provide recommendations on service contracts and organize the logistics for the repair of the equipment. Acquires specifications and quotes from suppliers
- Serve as the Research Scientist representative on the Department of Chemistry X-ray Crystallography Users committee
- Participate with the X-ray Crystallography Users Committee in preparation of grant proposals to acquire funding for new x-ray instrumentation, assesses equipment available from various vendors of the desired equipment and involved in negotiating terms of the purchase
- Handle the day-to-day operation including the management and supervision of the X-ray
  Crystallography Laboratory facility as well as the ordering of any supplies needed to run the X-ray
  equipment including x-ray tubes, etc.
- Ensure our licenses are up-to-date for the Cambridge Crystallographic Database and the Inorganic Crystal Structure Database



- Update and maintain the X-ray Crystallography Laboratory/Facility website content including offering electronic sample submission
- Keep electronic records of billing information to forecast activity in the facility.

## Financial Administration of the X-ray Crystallography Laboratory

- Ensure that the X-ray Crystallography Laboratory operates on a revenue neutral basis with all
  expenses associated with repair, maintenance and consumables being offset by charges to users
- Establish pricing policy for the services provided by the facility with approval from the Department Chair and X-ray Users Committee and review the fee structure on an annual basis
- Responsible to billing of users and submit the monthly internal charges to the Department Financial Officer for processing and to invoice external clients for all worked done in the facility
- In collaboration with the Department Financial Officer and Administrative Officer, provides input into the annual operating budget needed to operate the facility
- Responsible to submit equipment consumables and repair cost requisitions through Unit 4

#### **Training**

- Prepare user guides and procedures for standard operations of the X-ray equipment
- Train non-specialized users on X-ray equipment which includes new graduate students and postdocs plus faculty and staff from across campus. Each user must receive extensive training before access to the equipment can be granted. Also provides technical support during the use of equipment after training has occurred.
- Instruct groups with varying degrees of requirements, providing individualized training as necessary
- Provide each user with safety training for working with X-ray equipment

## X-ray Crystallography Laboratory/Facility Maintenance Work

- Maintain the safe operation of the X-ray equipment. This includes changing the X-ray tube every couple of years, cleaning the cooling system, calibrating the equipment, upgrading the software, etc.
- Run periodic performance checks on the X-ray equipment as a requirement of compliance and to ensure all instruments are maintained at peak performance
- Use sound judgement for preliminary diagnosis of X-ray equipment malfunctions and repairs

#### Safety

- Responsible for safety in the laboratory, ensuring that procedures with regard the X-ray machine which is high voltage equipment
- Maintain personal certifications as required by the Safety Office
- Update posted safety procedures including WHMIS, hazardous waste disposal etc. so that they are current
- Maintain equipment certifications and the associated records
- Prepare and maintain current Standard Operating Procedures (SOPs)
- Maintain first aid kits
- Complete monthly safety inspections using Safely and report unsatisfactory reports to the Department and Safety Office as required
- Ensure adherence to Health and Safety guidelines by all users

#### Other

- Keep abreast of new developments in techniques and instrumentation in X-ray crystallography and implement the techniques in the X-ray facility as time and budget permits
- Participate in conferences to stay current on X-ray crystallography technology and techniques keeping the facility state of the art
- Serve as a Research Scientist technical resource person for faculty, research associates, PDFs, and students in the development of their research projects



\*All employees of the University are expected to follow University and departmental health and safety policy, procedures and work practices at all times. Employees are also responsible for the completion of all health and safety training, as assigned. Employees with staff supervision and/or management responsibilities will ensure that assigned staff abide by the above, and actively identify, assess and correct health and safety hazards, as required.

#### **Required Qualifications**

#### Education

Ph.D. in Chemistry Chemical Crystallography is required

## **Experience**

 At least 5 years' experience in working with X-ray Crystallography equipment. Must be highly trained and knowledgeable about the Physics, Crystallography and all branches of Chemistry including Organic, Inorganic, Organometallic, Solid state Chemistry, etc.

### Knowledge/Skills/Abilities

- Strong understanding of Crystallography, Chemistry and Physics
- Working knowledge and trained in providing solution and refinement of crystal structure of solids
- Knowledge of safety procedures for X-ray equipment is required.
- Proven ability to maintain and repair the X-ray equipment and communicate with users
- Ability to manage multiple priorities in a fast-paced environment is essential
- Excellent written and oral communication skills required
- Advanced experience with Microsoft Office Suite, Crystallography Software, etc. required
- Advanced computer skills including Unix-based programming required
- Incumbent must also complete all required safety training modules as per Safety Office Regulations (e.g., WHMIS, Laboratory Safety, Employee Safety Training, Workplace Violence Awareness Program, and HRs Accessibility module).

#### **Nature and Scope**

- Contacts: Significant internal relationships include Department Chair and Associate Chairs, Department of Chemistry X-ray Crystallography Users Committee, Chemistry faculty, graduate students, undergraduate students and research personnel, Faculty, staff and students across the Faculties of Science and in other units (e.g. Engineering). Significant external relationships include suppliers (e.g. Bruker), Science Technical Services, Plant Operations and external user such as other Canadian Universities and industry.
- Level of Responsibility: Must be able to work independently. The position has very specialized work with no supervision and provides technical advice and guidance to others. Oversee the day-to-day operation of highly specialized equipment under the jurisdiction of the Department of Chemistry X-ray Crystallography Users Committee. An error in the use of the equipment can result in serious damages to the X-ray equipment.
- Decision-Making Authority: The incumbent will make recommendations on service contracts and new instruments in the X-ray Crystallography Facility. The Research Scientist participates with the X-ray Crystallography Users Committee in preparation of grant proposals to acquire funding for new x-ray instrumentation, assesses equipment available from various vendors of the desired equipment and involved in negotiating terms of the purchase. The Research Scientist is also involved in the annual budget planning process with the Department Financial Officer and Administrative Officer providing input on the annual budget needed to run the facility.
- Physical and Sensory Demands: Attention to detail is needed. High voltage, X-ray radiation, Chemical compounds, Solvents, etc..



• Working Environment: Some (e.g. over Christmas break) holiday hours are required to check the status of the laboratory. After hours sometimes required for coming to the Facility to stop the experiment, stop liquid nitrogen, etc.