

## ***Openings for Ph.D. students:***

INTERPRETING DIFFUSE SCATTERING FROM DISORDERED MATERIALS:  
DEVELOPMENT OF MODELS AND TESTING OF SOFTWARE WITH  
SUPERCOMPUTERS

*Summary of Research Plan.* Develop structure elucidation at the nano- to micrometer length scales for materials that may have interesting properties due to a lack of structural order. The research involves testing efficient conceptually revolutionized software for interpreting diffuse neutron and X-ray scattering data, with the help of supercomputers.

*Objectives and methods.* The objective of this project is to transform current heuristic approaches for analyzing the total, three-dimensional diffraction pattern (including non-Bragg scattering) of solid-state materials into a unified, efficient and conceptually revolutionized computational method that capitalizes on (a) new technologies in large-scale computing, (b) a new crystallographic description of disordered crystal structures, (c) progress in modeling molecular and other materials, and (d) advances in synchrotron and neutron physics. We are designing efficient computer programs that will be tested on real data with the help of the world-class high-performance computing facility of the National Center for Computational Sciences at Oak Ridge National Laboratory (ORNL) and the grid computing facility associated with the Institute of Organic Chemistry of the University of Zürich (UZH).

The project is multi-disciplinary and involves an international team effort between the University of Zürich, ETH Zürich and ORNL. The project is further motivated by the single-crystal diffraction facility TOPAZ being built at the Spallation Neutron Source at ORNL, and by the planned upgrades of the European Synchrotron Radiation Facility (ESRF) in Grenoble, France.

***Openings*** are available for ***Ph.D. students*** (workplace ORNL) with a solid background/interest in solid state physics, X-ray and neutron diffraction and a demonstrated ability to learn quickly new concepts and theory. The positions are part of a Sinergia project funded by the Swiss National Science Foundation. Please send applications, together with 2 letters of recommendation to:

*Professor Kim Baldridge* (kimb@oci.uzh.ch), +41 (0)44 635 4201, Institute of Organic Chemistry, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland.