For a project re-defining data quality assessment in single-crystal diffraction, the Thorn Group at the Rudolf Virchow Center for Experimental Biomedicine of the University of Würzburg is searching for a

**Postdoctoral Researcher (m/f/d)**

**Scope and your role**
You will undertake research in the group of Dr. Andrea Thorn to improve the quality of measurements and processing of XFEL, neutron and conventional X-ray diffraction data, to establish major error sources and to define new best practices for macromolecular diffraction experiments. We aim to create new automatic and visual diagnostics by expanding the AUSPEX software ([www.auspex.de](http://www.auspex.de)) using statistical analysis, machine learning and visual data representation. In order to do so, collaboration was set up with four major diffraction facilities in Europe: the BESSY synchrotron in Berlin, the European Spallation Source (ESS) in Lund, the ESRF in Grenoble as well as the European XFEL in Hamburg. You will visit these facilities regularly to develop and implement new diagnostics in close collaboration and publish your results in peer-reviewed journals. Furthermore, you will be expected to contribute to teaching, training, public outreach and to present your work at in-house and international meetings.

This exciting project will allow you to define new quality standards in macromolecular structure determination and to establish a European network in the crystallographic community. Our group is well-connected and AUSPEX is part of the CCP4 suite for macromolecular crystallography. We maintain close ties with other method developers worldwide.

**What we offer**
We offer a 30-month full- or part-time position at the Rudolf-Virchow Center (RVZ) of the University Würzburg, the birthplace of X-rays, with a competitive salary commensurate with your training and experience according to salary agreement TV-L. Your position is funded by the German Federal Ministry of Education and Research (BMBF) as part of the AUSPEX project.

You will have access to both national and the public-service pension schemes (VBL), health care, and 30 days of holiday entitlement (if working full-time) in addition to 13 annual public holidays in Bavaria. The University also offers access to employee shopping/travel discounts, and there might be cake on occasion. The JMU Welcome Center supports international candidates with finding accommodation, general information regarding taxes, insurance, healthcare and other administrative matters. The University also offers support for candidates with children, including the University kindergarten, advice regarding school placement, holiday programs and flexible work hours.
Qualification profile
You should have a doctoral degree in a chemical, biological, physical, computational or other relevant subject or be due to complete your doctoral studies within 3 months of applying. You should be able to develop your own ideas, and have the necessary skills to successfully drive and complete a research project, both working independently and as part of a team.

We are looking for someone with a good working knowledge of Linux, Python and C++, ideally including common crystallographic libraries such as gemmi, cctbx or clipper. You should be good at statistical data analysis, ideally including experience with the statistical package R. Web-based programming skills (e.g. JavaScript, html5, css), previous experience with machine learning and neural networks are also a bonus. You should have previous experience in crystallography or be willing to learn both its theoretical basis as well as how to conduct crystallographic experiments on the job.

You should be a good communicator, willing to convey complex problems to lay audiences, as well as to instruct and supervise students. An excellent command of English is a prerequisite; German language skills will also be required, but if you do not speak German, we will offer training. Due to the collaborative nature of this project, you should be willing to travel.

Female scientists are particularly encouraged to apply! Disabled applicants will be preferentially considered in case of equivalent qualification.

The position will start on September 1st, 2019 or later. Applications should be sent by e-mail as one single pdf-document including: cover letter, curriculum vitae (including software projects you contributed to, teaching experience and academic track-record), diplomas/certificates and 3 addresses of referees by August 31st, 2019 to andrea.thorn@uni-wuerzburg.de.

If you have any further questions, please do not hesitate to contact us!

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Lap page: www.uni-wuerzburg.de/rvz/forschung/assozierte-forschungsgruppen/ag-thorn/