Graduate Student / Researcher (1 year)  
Advanced Discovery of Materials Structure

Discovery of new materials for energy and sustainability applications relies on characterization of materials at the atomic scale. Analysis of experimental observation depends on accuracy of data modelling. Here we devise new methods to overcome current limitations in analysis of scattering data. The announced position is dedicated to the development of two segments of a software application, scientifically appealing and application oriented in the broad fields of chemistry and materials science:

• **Massively parallel library for solution of the Debye scattering equation**
  We develop an open-source library for efficient solution of the Debye scattering equation, which is capable of exploiting a wide scenario of hardware architectures. We will explore the possibility to use the library as plug-in within third-party software packages such as: LAMMPS, DISCUS, and PM2K.

• **Scattering Tool to Advance Research of Materials Structure**
  We develop a modern graphic-interface framework, which provides an easy control of complex analysis parameters. Oriented to user audience with little to none computational knowledge (e.g., laboratory experimentalists), the new application will serve future method developments, while working as interface with third-party simulation tools.

**Candidate profile**
You are highly motivated and you are deeply committed to research. You are able to work independently and as part of a team. You are equipped with an analytical and critical mind-set and you communicate clearly and concisely.

**Qualification**
• You have (or are expected to discuss within a year) a master degree in physics or related subjects.
• You have background in computational physics
• You have experience in software development (C/C++ (mandatory), Python (optional))

**Application**
Send a brief letter of interest to Dr. Alberto Leonardi (alberto.leonardi@fau.de) with:
• Short cover stating your past experience on software development
• CV including eventual publication list
• Reference list (optional)
The position will be open until it is filled.

**Fund**
The position is founded through KONWHIR program at RRZE center.

**Further information**
Feel free to contact Dr. Alberto Leonardi (alberto.leonardi@fau.de) for any question about this post (e.g., project details, qualifications, type of position, etc.).