**2017 Helmholtz – OCPC – Programme**

**for the involvement of postdocs in bilateral collaboration projects**

**PART A**

**Title of the project:**

**Nonlinear ultrafast x-ray spectroscopy to study charge transport in molecular systems**

**Helmholtz Centre and institute:**

**DESY Deutsches Elektronen-Synchrotron**

**Project leader:**

**Prof. Dr. Nina Rohringer**

**Web-address:** http://www.mpsd.mpg.de/en/research/qox

**Description of the project:**

X-ray free-electron laser (FEL) sources are relatively new accelerator-based x-ray sources that provide x-ray pulses of ultrashort (femtosecond) duration and ultrahigh intensities. Also China is advancing in the field, with the recent opening of the Dalian VUV FEL facility and anticipated projects to build a hard x-ray FEL in Shanghai. With unprecedented intensities that are achievable by focusing FEL beams (up to 1020 W/cm2 for hard x-rays), stimulated and nonlinear x-ray matter interaction becomes accessible in experiments, resulting in effects like multiple sequential photoionization, strong coherently amplified spontaneous x-ray emission by stimulated emission, stimulated inelastic x-ray scattering, parametric sum frequency conversion and dynamical interference in photoionization, to name a few. In particular, our group could demonstrate stimulated x-ray emission in a variety of targets, ranging from gases of single atoms, molecules, liquids to thin films and clusters. By studying the spectral characteristics of stimulated x-ray emission over amplification ranges of 4 orders of magnitude and different samples, we recently could also demonstrate, that the chemical sensitivity of the characteristic x-ray emission seems to be pertained. Despite the high amplification gains and necessary x-ray intensities on target, the spectral output is not modified by radiation damage of the sample. This finding sets the scene for the extension of powerful nonlinear spectroscopies from the optical to the x-ray domain that will allow for probing the time dynamics of electronic wave packets in molecular systems and study effects such like coherent, long-range charge transfer in biological molecules with unprecedented temporal and spatial resolution. Although the basic ideas of nonlinear x-ray spectroscopy have been developed previously, a critical case study and theories that are matched to realistically achievable FEL-pulse properties need to be developed. We offer a postdoc position in our group to develop a quantitatively predictive theory for nonlinear x-ray spectroscopy, based on sequence of two broadband x-ray pulses that stimulate resonant inelastic (Raman) x-ray scattering in a molecular target. In particular, charge-transfer processes and charge migration in smaller molecular systems and molecular chains will be studied, that still allow for the self-consistent treatment of the electronic and nuclear motion, along with the changes of the spectral properties of the applied x-ray fields. The project will involve the use and development of quantum chemistry codes that allow for the calculation of time-dependent electronic and nuclear properties. Furthermore a general electronic/nuclear density-matrix approach will be developed that can be efficiently coupled to Maxwell’s equations, to predict the outgoing x-ray fields in a quantitative matter. The goal of the project is to provide a detailed feasibility study of nonlinear x-ray spectroscopy at current and future x-ray FEL sources and to define the x-ray pulse parameters that are needed for a successful experiment. The offered theoretical/computational projects will be in close connection to experimental campaigns at x-ray free-electron laser (XFEL) facilities and in collaboration with experimental groups, and the applicant will also have the opportunity to participate at experimental campaigns (online data analysis) at these fascinating and powerful x-ray sources, in particular the European XFEL on the DESY campus, that will start operation in this year.

**Description of existing or sought Chinese collaboration partner institute:**

Interested candidates from the Department of Modern Physics, University of Science & Technology of China (USTC), the Institute of Applied Physics & Computational Mathematics (IAPCM), the Institute of Physics of the Chinese Academy of Science, or Fudan University Shanghai are especially welcome to apply.

**Required qualification of the post-doc:**

* Applicants are expected to have an excellent track record and a PhD in physics or physical chemistry, and excellent skills in spoken and written English. A strong record and interest in programming and code development in C++ is expected. We are looking for highly motivated individuals with a background in theoretical atomic or optical physics, theoretical solid-state physics, quantum optics, quantum chemistry, x-ray science, strong-field physics or related fields.
* Experience in one or several of the following areas is highly desirable: numerical physics, development of quantum chemistry codes, x-ray spectroscopy, electronic structure calculations, Auger spectroscopy, nonlinear optical spectroscopy, physics of clusters

**PART B**

**Documents to be provided by the post-doc:**

* + Detailed description of the interest in joining the project (motivation letter)
  + Curriculum vitae, copies of degrees
  + List of publications
  + 2 letters of recommendation

**PART C**

**Additional requirements to be fulfilled by the post-doc:**

* Max. age of 35 years
* PhD degree not older than 5 years
* Very good command of the English language
* Strong ability to work independently and in a team