**2018 Helmholtz – OCPC – Program**

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

**DESY\_OCPC\_2018-11**

**PART A**

**Title of the project:**

Development of atomic electronic structure theory in solid-density plasma driven by intense x-ray free-electron laser pulses

**Helmholtz Centre and Research Group: DESY**

**Project leader:**

Prof. Dr. Robin Santra, DESY and University of Hamburg

Dr. Sang-Kil Son, DESY

**Web-address:**

https://desy-theory.cfel.de

**Description of the project** (max. 1 page)**:**

X-ray free-electron lasers (XFELs) open a new era in science and technology, offering unique opportunities that have not been conceivable with conventional light sources. Research areas such as plasma and warm dense matter physics or coherent x-ray imaging take advantage of the unprecedentedly high intensities of XFELs. A single XFEL pulse can induce very complex dynamics within matter initiated by core-hole photoionization. Due to this complexity, it is important to describe detailed dynamical behavior of matter when it is exposed to intense x-rays. Several ground-breaking experiments and theoretical developments over recent years have been carried out along with the consecutive launch of large-scale XFEL facilities around the world, and more facilities, including the Shanghai XFEL in China, will come out soon and bring breakthroughs in the next generation of XFEL applications.

The CFEL-DESY Theory Division led by Prof. Dr. Robin Santra is one of the worldwide leading groups in XFEL science. We have significantly contributed to cutting-edge theoretical development for XFEL-matter interaction and software development for describing dynamical behavior of atoms, molecules, and complex systems interacting with intense x-ray pulses. Our theoretical models have been verified through a series of successful demonstrations [1-3], and our tools have played a key role in interpreting XFEL experimental data and designing new experiments. The electronic structure of matter at high x-ray intensity is the essence of our theoretical framework. Based on atomic electronic structure calculations, XATOM—an x-ray atomic physics toolkit—calculates atomic data (cross sections and rates) of x-ray-induced atomic processes, which are used not only for simulating atomic ionization dynamics, but also as input for XMDYN —a Monte Carlo molecular-dynamics-

based code—for simulating complex systems irradiated by intense XFEL pulses. XMDYN combined with XATOM has served as the essential tool for describing complex systems such as fullerene molecules, noble gas clusters, and so on [4].

In the proposed project, we will develop a better description of atomic electronic structure in x-ray-driven condensed matter. Most plasma-simulation codes utilize atomic data calculated within an isolated atom model. The electronic structure for an atom embedded in a dense plasma might be affected by the local plasma environment. To treat a bulk system, it is desirable to employ periodic boundary conditions with supercells in XMDYN simulations. We plan to extend our tools such that the atomic electronic-structure calculation (XATOM) takes into consideration, for every atom in the supercell, the local plasma environment as simulated using XMDYN. In this way, we will develop a new simulation tool that should be able to quantitatively predict the dynamics of x-ray-induced warm-dense-matter production, including a dynamical description of what is known as ionization potential depression. With this newly developed tool, we will be able to further explore non-equilibrium dynamics of matter under extreme conditions and coherent diffractive imaging of biological macromolecules.

[1] B. Rudek *et al.*, *Nature Photonics* **6**, 858 (2012).

[2] B. Murphy *et al.*, *Nature Communications* **5**, 4281 (2014).

[3] A. Rudenko *et al.*, *Nature* **546**, 129 (2017).

[4] Z. Jurek *et al.*, *Journal of Applied Crystallography* **49**, 1048 (2016).

**Description of existing or sought Chinese collaboration partner institute** (max. half page):

In order to quantitatively describe excitation and relaxation dynamics in matter, *ab initio* electronic structure theory is the key ingredient. We seek expertise in quantum many-body theory for atoms and molecules, interaction between light and matter, and warm dense plasma physics. Recently, the Department of Physics and Center for Atomic and Molecular Nanosciences at Tsinghua University has demonstrated a simulation of XFEL-driven warm dense plasma of aluminum with accurate atomic data, including ionization potential depression calculated by dedicated density functional theory method. This work for light atoms could be a benchmark for our projected work and a starting point to investigate complex systems containing heavy atoms. The advent of the Dalian VUV FEL and the Shanghai XFEL raises the need of a detailed understanding of x-ray-matter interaction and expertise in XFEL-driven science in China. Collaboration with Tsinghua University will be a first step towards further theoretical development of studying XFEL-induced warm dense matter and future advances in XFEL science.

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

* PhD in physics and related fields
* Experience with electronic structure theory and atomic and/or plasma physics
* Additional skills in scientific code development and data processing

**PART B**

**Documents to be provided by the post-doc, necessary for an application to OCPC via a postdoc-station:**

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

**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