

Science at X-ray Free Electron Lasers

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X-ray Free Electron Lasers (FELs) deliver coherent X-ray pulses, combining unprecedented power densities of up to 1020 W/cm² and extremely short pulse durations down to hundreds of attoseconds. Such intense X-ray FEL pulses make single-shot diffraction of nanometer-size objects, tiny protein crystals, and non-crystallized biomolecules a tangible reality. Such ultrashort X-ray FEL pulses allow us also to visualize femtosecond-scale temporal variations of charge and structure that may occur upon photoexcitation in any form of matter. On the other hand, since the X-ray FEL pulses give access to a new regime of X-ray intensities, they open new venues in studying the interaction between intense X-rays and various forms of matter. Understanding the ultrafast reactions induced by the X-ray FEL pulses is of fundamental interest, as well as of crucial importance, for the X-ray FEL applications.

There are seven short-wavelength FEL facilities in operation in the world. The first FEL facility FLASH (the Free Electron LASer in Hamburg) in Germany started operation for users in 2005. It provides FEL pulses in the range of extreme ultraviolet to soft X-rays. The first hard X-ray FEL facility LCLS (the Linac Coherent Light Source) in the United States of America started user operation in 2009. In 2012, the second hard X-ray FEL SACLA (the Spring-8 Angstrom Compact free electron LASer) in Japan and the first fully coherent seeded FEL FERMI (the Free Electron laser Radiation for Multidisciplinary Investigations) in Italy started user operation. In 2017, PAL-XFEL (the Pohang Accelerator Laboratory X-ray Free Electron Laser) in Korea, European XFEL (European X-ray Free Electron Laser), SwissFEL (Swiss X-ray Free Electron Laser), and DCLS (the Dalian Coherent Light Source) in China started operations.

Following the success of the first Special Issue *X-ray free electron laser*, we have edited the second Special Issue *Science at X-ray free electron lasers*. This Special Issue aims to cover recent developments of XFELs and sciences there, focusing on new beamlines, end stations, and operating modes, as well as relevant theoretical studies. For this purpose, this special issue collected the following articles.

Where the variable gap undulators were installed, FLASH2 has been run simultaneously with FLASH1 since 2016. Here, Robert Moshhammer and coworkers successfully reinstalled Reaction Microscope, which allows us to record three-dimensional momenta of all electrons and ions ejected from a single atom or molecule simultaneously, as described by Meister et al. [1] together with some beautiful science cases studied by this end station.

At European XFEL, the first high-repetition-rate Hard X-ray FEL in the world, Christian Bressler and coworkers successfully installed femtosecond X-ray experiments (FXE) instrument that allow us to study various kind of ultrafast X-ray photochemistry, as described by Khakhulin et al. [2], whereas Adrian Mancuso and coworkers successfully installed the single particles, clusters, and biomolecules and serial femtosecond crystallography (SPB/SFX) instrument with a wide range of options of sample deliveries, which allow us to perform various class of structural biology experiments, as described by Mills et al. [3] together with some beautiful showcase examples. Gianluca Geloni and coworkers have been working on the installation of an X-ray pump and X-ray probe system in the soft



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X-ray SASE3 beamline, as an upgrade project, and Serkez et al. describes this project in ref. [4].

At SACLA, the second-oldest hard X-ray FE in the world, there are a few new instrumentations and developments to be noted. Nango et al. [5] describes a current status of pump-probe time-resolved serial femtosecond crystallography for photosensitive protein molecules, as a holy grail of X-FEL science. Inubushi et al. [6] describes a recent development of experimental platform for combinative use of an X-ray FEL and a high-power nanosecond laser for investigating matter in extreme conditions. Yumoto et al. [7] describes state-of-the-art nanofocusing optics for an X-ray FEL generating an extreme intensity of 10^{20} W/cm², with a focus size of 210 nm × 210 nm, a pulse duration of 7 fs, and a pulse energy of 150 µJ (1/4 of the pulse energy generated at the light source), using total reflection elliptically figured mirrors, based on Kirkpatrick–Baes geometry. Nishiyama et al. [8] established simultaneous measurements of small-angle X-ray scattering, X-ray fluorescent photons, and ions ejected from nanoparticles that consists of xenon atoms and clearly demonstrated correlations of the size of nanoparticles and yields of fluorescence and ions. Claudiu et al. [9] employed focused X-ray FEL pulses to generate shock waves in the liquid water microdroplets and determined time-pressure histories of shocks, taking an advantage of very stable operation of SACLA.

Besides these recent developments and new science cases studied in the three focused FEL facilities, Cho [10] beautifully reviewed a status of X-ray spectroscopies of high energy density matter created with X-ray FELs generated at few facilities, Fadini et al. [11] discussed applications and limits of time-to-energy mapping of protein crystal diffraction using energy-chirped polychromatic X-ray FEL pulses, and Yuan and Bandrauk [12] discussed how to probe attosecond electron coherence in molecular charge migration by ultrafast X-ray photoelectron imaging, one of the hottest subjects in X-ray FEL science.

I hope this Special Issue will be helpful in providing useful information about the current statuses of the XFEL facilities and sciences that can be explored there, as well as future directions of this research field.

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