

## 2025 Helmholtz – OCPC – Programme for the involvement of postdocs in bilateral collaboration projects

### PART A

**Title of the project:**

Convergent-beam space-time-resolved X-ray crystallography

**DESY Division & Group:**

FS-CFEL-1, Coherent imaging division

**Project leader/supervisor:**

Chufeng Li and Henry Chapman

**Web-address:**

<https://cid.cfel.de/team/>

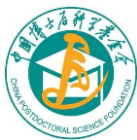
**Programme Coordinator** (Email, telephone and telefax)

Martin Sandhop; martin.sandhop@desy.de; +49 40 8998 4172

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

Using new multilayer Laue lenses (MLLs) developed at DESY, it is now possible to focus X-rays to spot sizes of several nanometers with high numerical aperture. In this project we will explore novel coherent diffraction and imaging methods using the convergent X-ray beam in various schemes.

- 1) When a macromolecular crystal is placed in focus, the Bragg orders that are usually observed are spread out and interfere with each other. This interference directly encodes the phases of the diffraction orders, but is sensitive to the relative position of the focus to the crystal lattice. Algorithms originally developed for ptychography or image classification will be used to determine these positions and extract the diffraction phases used to synthesize 3D molecular images.
- 2) When the crystal is placed far out of focus, there is a correlation between the location of the intersection of a ray with the crystal and its angle of incidence, which allows for the formation of 3-dimensional diffraction topograph for the crystal with high-precision indexing. Correcting the signals by the position-dependent diffraction efficiency improves the accuracy of crystallographic analysis for structure determination. Moreover, this unique capability offers space-resolved structural information during processes within the crystal.
- 3) When the ultra-short hard X-ray pulses (e.g. from X-ray free electron lasers) are focused by MLLs, X-rays illuminating the crystals at different incidence angles arrive at the crystal with different delay times determined by the path lengths in the focusing optics. This unique mechanism encodes the time-resolved information into the diffraction pattern with the resolution down to attosecond level. This will be developed for the investigation of chemical reactions.



The project will explore these aspects of convergent-beam diffraction utilising synchrotron sources and the European XFEL. Candidates will contribute to these experiments and develop algorithms and analysis methods to solve the molecular structure as well as the crystal structure and defects. The multiscale X-ray imaging methods described above are to be applied in both materials and life sciences.

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

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Institute of Physics Chinese Academy of Sciences (IOP)

IOP is the leading research institute in China in condensed matter physics and related fields. Through more than 90 years of development, IOP has become a comprehensive and multi-disciplinary research organization engaged in research on basic and applied physics. Its current research activities concentrate on condensed matter physics, optical physics, atomic and molecular physics, plasma physics, soft matter physics, and condensed matter theory and computation physics. More Information about IOP can be found at [www.iop.cas.cn](http://www.iop.cas.cn). Notable for this project is the operation of large-scale facilities and in particular the Dream Line - Shanghai Synchrotron Radiation Facility in Shanghai. As a consequence there are strong groups in crystallography, diffraction physics, and coherent diffractive imaging techniques.

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**Required qualification of the postdoc:**

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- A PhD in biophysics, biochemistry, structural biology, or similar
- A strong background in diffraction physics, crystallography, or X-ray optics.
- Proficiency in scientific programming and computation using Python, Bash, Matlab, and C/C++.
- Experience in algorithm and scientific software development.
- Self motivated and works well in an interdisciplinary team environment
- Excellent interpersonal skills and a friendly nature
- Good communication skills in English