

HeXI: The High-energy Electron Xtallography Instrument

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The High-energy Electron Xtallography Instrument (HeXI), currently under construction at Diamond, aims to significantly broaden the range of samples suitable for structure determination by electron diffraction. Funded by the Wellcome Trust “Electrifying Life Sciences” grant and Diamond Light Source, the HeXI project will leverage the increased penetration of Mega-electron-volt (MeV) electrons to bridge the crystal size gap between electron and X-ray scattering, enabling the determination of structures from crystals ranging between 300 nm and 3 μm .

A tuneable electron source, operating between 100 kV and 1 MeV, will be used to explore improvements in data fidelity arising from reduced dynamical scattering and a more kinematic scattering regime. HeXI will combine the unique sensitivity of electrons to structural information with the advanced goniometry developed at Diamond for macromolecular X-ray crystallography, reducing measurement geometry instabilities and enhancing overall data quality.

HeXI will offer data collection in three distinct modalities:

1. Three-dimensional electron diffraction (3DED) of small molecules – Structure determination of small molecule structures from chemical syntheses, without significant further purification or crystallization.
2. Cryo-3DED/microED of proteins – Structure determination from frozen-hydrated protein crystals which are too small for traditional MX.
3. SerialED – Time-resolved (ms to μs) structure determination of protein crystals.

This talk will present a progress update on the HeXI project and discuss the capabilities of this novel instrument, highlighting the potential to transform the field of macromolecular structure determination.