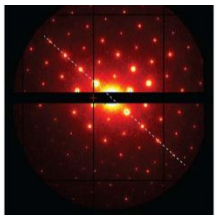

Megaelectronvolt Ultrafast Electron Diffraction at PolFEL:

Building a World-Leading Facility for Structural Dynamics in Poland

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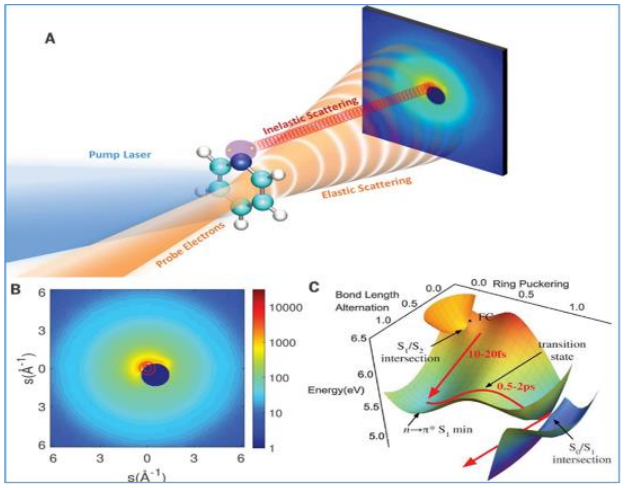
Megaelectronvolt Ultrafast Electron Diffraction (MeV-UED) is a pump-probe technique that uses relativistic electron pulses to capture structural snapshots of matter with femtosecond temporal and sub-Ångström spatial resolution. Relativistic electrons offer key advantages over keV-class sources: space-charge effects are strongly suppressed enabling shorter, denser bunches; velocity mismatch with the optical pump is negligible; and the flat Ewald sphere at MeV energies provides simultaneous access to a wide range of momentum transfers.

This talk introduces the principles of MeV-UED and surveys its scientific applications — from real-time imaging of chemical bond dynamics in gas-phase molecules [1], through charge-density-wave and phase-transition dynamics in quantum materials, to microcrystal electron diffraction (MicroED) of organic and pharmaceutical compounds.



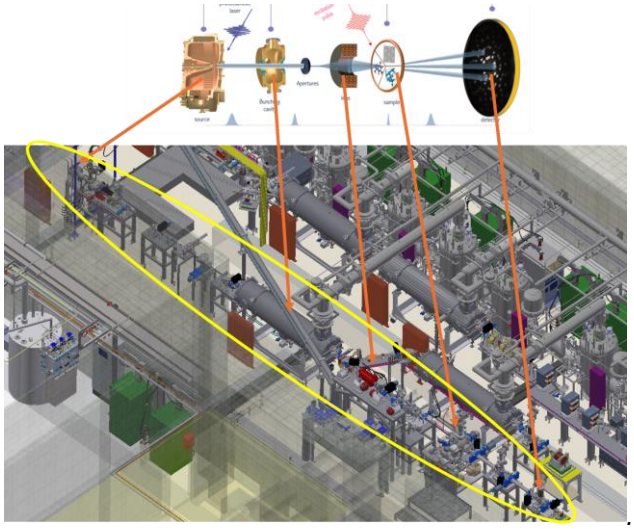


Fig. 1 ***A)*** *Pump–probe schematic — elastic (orange) probes nuclei, inelastic (red) probes valence electrons.* ***(B)*** *Diffraction pattern.* ***(C)*** *Pyrazine S_1/S_2 potential-energy surface.[1]. Fig. 2 MeV-UED beamline geometry — photocathode source, bunching cavity, aperture stack, focusing lens, sample chamber, and pixelated detector.*

The second part of the talk focuses on PolFEL, a Polish accelerator-laser based user facility currently under construction at NCBJ Świerk. PolFEL's MeV-UED beamline, driven by a superconducting RF linac, could operate at repetition rates up to 1 MHz — orders of magnitude beyond existing facilities — unlocking statistical regimes currently inaccessible: serial crystallography datasets in seconds, access to weakly scattering systems, and high-fidelity diffuse scattering. We discuss the instrument design, expected performance parameters, and scientific opportunities — with particular attention to structural chemistry and quantum crystallography applications relevant to the University of Warsaw research community.

1. An example from: Yang, J., Zhu, X., F. Nunes, J. P., Yu, J. K., Parrish et al., (2020). Simultaneous observation of nuclear and electronic dynamics by ultrafast electron diffraction**.** ***Science***, *368*(6493), 885–889