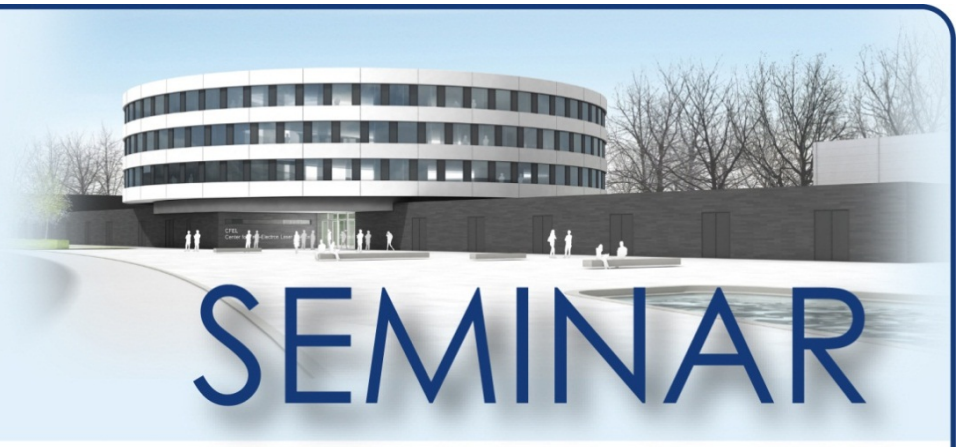
CFEL SCIENCE



SEMINAR

11th September 2024 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

Sourav Banerjee

Center for Free-Electron Laser Science, DESY, Hamburg, Germany

Plasma environmental effects on the radiation damage in X-ray nanocrystallography

The availability of high intensity and ultrashort X-ray pulses from X-ray free-electron laser (XFEL) sources have opened the possibility of imaging nano-sized biological samples, i.e., single particles (such as a macromolecule or a virus) and nanocrystals. Though the principle of diffraction before destruction is underlying the concept of structure determination at high X-ray intensities, radiation damage is nonetheless a limiting factor. The plasma produced within the sample due to ionization and subsequent photoinduced processes enhances significantly the degree of damage in the sample, i.e., via collisional ionization. In this talk, results from theoretical simulations on a prototypical nanocrystal will be shown to demonstrate the determination of ionization potential depression (IPD) using a non-local thermal equilibrium (NLTE) approach combined with quantum mechanical electronic structure calculation. The impact of enhanced collisional ionization and radiation damage due to the inclusion of the transient IPD will also be discussed.

Host: Robin Santra – CFEL-DESY Theory Division