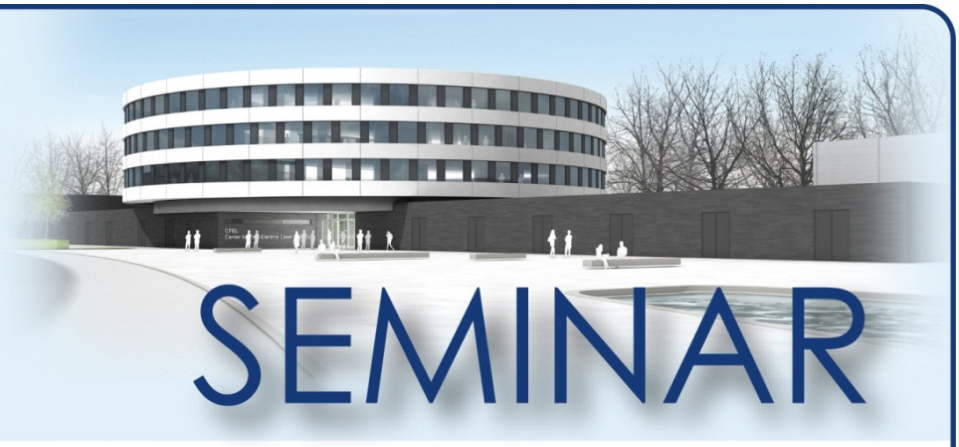
CFEL SCIENCE



SEMINAR

6th May 2020 - 2:00 p.m.

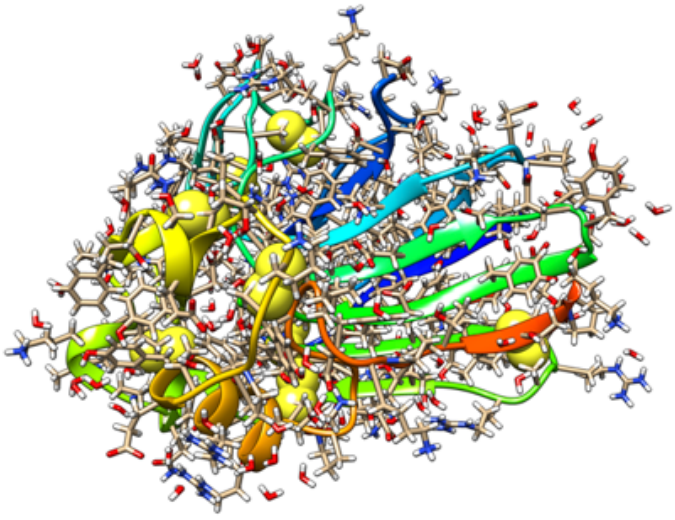
Virtual meeting room in ZOOM (ID: 960 9376 2874 / PW: 79361245)

Malik Muhammad Abdullah

Deutsches Elektronen-Synchrotron DESY, Germany

Femtosecond dissociation of disulfide bridges within XFEL irradiated protein crystals of Thaumatin

X-ray free-electron lasers (XFELs) enable crystallographic structure determination beyond the limitations imposed upon synchrotron measurements by radiation damage. Here we report a femtosecond time-resolved X-ray pump/X-ray probe experiment on protein nanocrystals of Thaumatin and Gd-Lysozyme. The correlated movements of sulfur ions were observed in XFEL-irradiated Thaumatin nanocrystals. We observe changes in the protein backbone and aromatic residues as well as disulfide bridges. Our in-house tool XMDYN was used for the simulations to look into the correlated structural dynamics in Thaumatin and was able to provide concrete description of the underlying dynamics as a function of time delay. Simulations show that the correlated structural dynamics are much slower than expected for the predicted high atomic charge states due to significant impact of ion caging and plasma electron screening and are in agreement with the experimental results. We decoupled our simulations for different conditions and pin point the origin of structural changes in Thaumatin nanocrystal. In this seminar we will go through the methodology of our simulations to explain XFEL pump/probe experiments for nanocrystal irradiation.



Thaumatin single-molecule, comprising of 8 disulfide bridges

Host: Robin Santra – CFEL-DESY Theory Division