CFEL SCIENCE

SEMINAR

20th March 2019 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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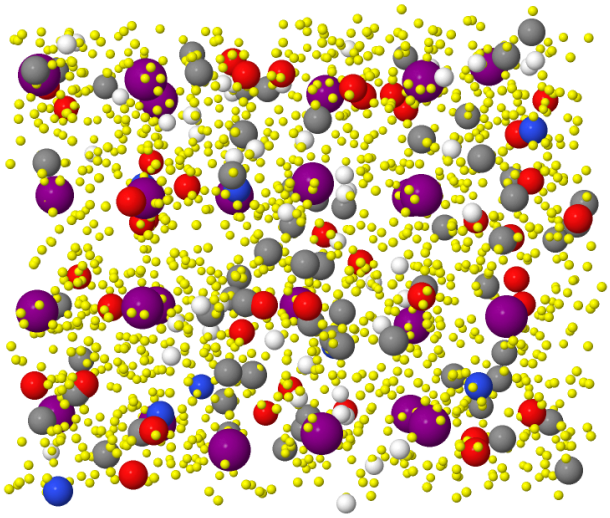
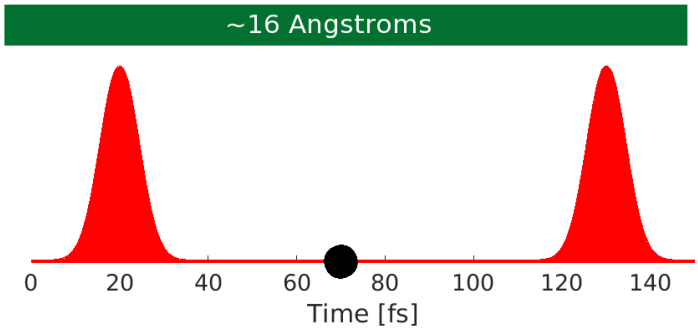
A simulation study of hard x-ray pump probe of I3C and Thaumatin nanocrystals

The standard method of reconstructing the structure of a protein is x-ray diffraction from its crystalline phase. X-ray free-electron lasers (XFELs) provide novel opportunities for bio-molecular structure determination. Due to the extreme intensity and ultrashort pulse duration of an XFEL pulse the diffraction technique is being extended towards nano size crystals and the ultimate goal is to reach the single molecule limit. XMDYN, a molecular dynamics/Monte Carlo code has been developed within the CFEL-DESY Theory Division during the past years. It has been extended to investigate the cumulative effect of representative sub-units of a nanocrystal experiencing different x-ray intensities. To demonstrate the efficacy of the methodology, I will present the simulated results of two experiments conducted at the LCLS on the progressive ionization damage in 5-amino-2,4,6-triiodoisophthalic acid (I3C) and Thaumatin nanocrystals.





Host: Robin Santra – CFEL-DESY Theory Division