CFEL SCIENCE

SEMINAR

18th June 2025 - 2:00 p.m.
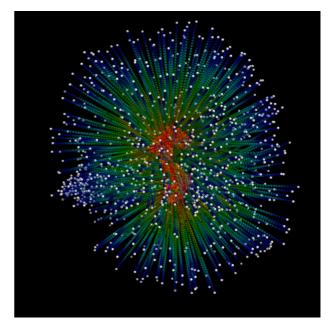CFEL-bldg. 99, seminar room IV

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Protein structure classification based on X-ray-laser-induced Coulomb explosion

We present simulations of Coulomb explosion dynamics due to fast ionization induced by high-intensity x-rays in six proteins that share similar atomic content and shape. We followed and projected the trajectory of the fragments onto a virtual detector, providing a unique explosion footprint. After collecting 500 explosion footprints for each protein, we utilized principal component analysis and *t*-distributed stochastic neighbor embedding to classify these. Results show that the classification algorithms were able to separate proteins on the basis of explosion footprints from structurally similar proteins into distinct groups. The explosion footprints, therefore, provide a unique identifier for each protein. We envision that method could be used concurrently with single-particle coherent imaging experiments to provide additional information on shape, mass, or conformation.

Host: Robin Santra – CFEL-DESY Theory Division