DAMOP16-2016-000654

Abstract for an Invited Paper
for the DAMOP16 Meeting of
the American Physical Society

Ultrafast ionization and fragmentation dynamics of molecules at high x-ray intensity

SANG-KIL SON, CFEL, DESY

X-ray free-electron lasers (XFEL) open a new era in science and technology, offering many unique opportunities that have not been conceivable with conventional light sources. Because of their very high x-ray photon fluence within very short pulse duration, materials interacting with XFEL undergo significant radiation damage — they possibly become highly ionized and then explode. To comprehend underlying physics, it is crucial to understand detailed ionization and fragmentation dynamics of atoms and molecules during intense XFEL pulses. We have developed the XMOLECULE toolkit to describe molecular x-ray-induced processes and to simulate radiation damage dynamics of molecules. In this talk, I will present a theoretical framework of XFEL-matter interaction, namely x-ray multiphoton absorption. Then I will discuss recent results of ultrafast x-ray-induced explosion of methyl iodide (CH_3I) molecules. Charge state distribution and kinetic energy releases of fragments are calculated to probe ionization and fragmentation dynamics, and compared with recent experimental results. It will be demonstrated that ionization of heavy-atom-containing molecules at high x-ray intensity is much enhanced in comparison with the isolated atomic case, due to ultrafast charge rearrangement during x-ray multiphoton absorption.