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

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Topic: F

X-ray free-electron lasers (XFELs) have brought an impact on various scientific fields, including AMO physics, material science, astrophysics, and molecular biology. Understanding how matter interacts with intense x-ray pulses is essential for most XFEL applications. Exposed to an intense x-ray pulse, an atom within a molecule absorbs many photons sequentially and ejects many electrons, turning into a highly charged ion within a femtosecond time scale. This multiphoton multiple ionization dynamics differs from that at a third-generation x-ray synchrotron radiation source, where one-photon absorption is dominant, and from multiphoton strong-field ionization, where many photons are simultaneously absorbed to ionize a single electron. The created charges are redistributed within the molecule, and then it explodes due to Coulomb repulsion. This fragmentation dynamics occurs along with ionization dynamics.

In this talk, I will present a theoretical framework to treat x-ray-induced processes and to simulate detailed ionization and fragmentation dynamics of atoms and molecules, introducing two dedicated x-ray physics toolkits, XATOM [1-4] and XMOLECULE [5-7]. With a joint experimental and theoretical study of small polyatomic molecules irradiated by XFEL pulses, I will demonstrate how the theoretical model describes the essential mechanisms underlying explosion dynamics of molecules in intense x-ray pulses. One of the key findings is that ionization of heavy-atom-containing molecules at high x-ray intensity is substantially enhanced in comparison with that of isolated atoms. This is called charge-rearrangement-enhanced x-ray ionization of molecules (CREXIM) [7] as illustrated in Figure 1. The CREXIM effect plays an important part in the quantitative understanding of XFEL–molecule interactions and will need to be taken into account for future XFEL applications.

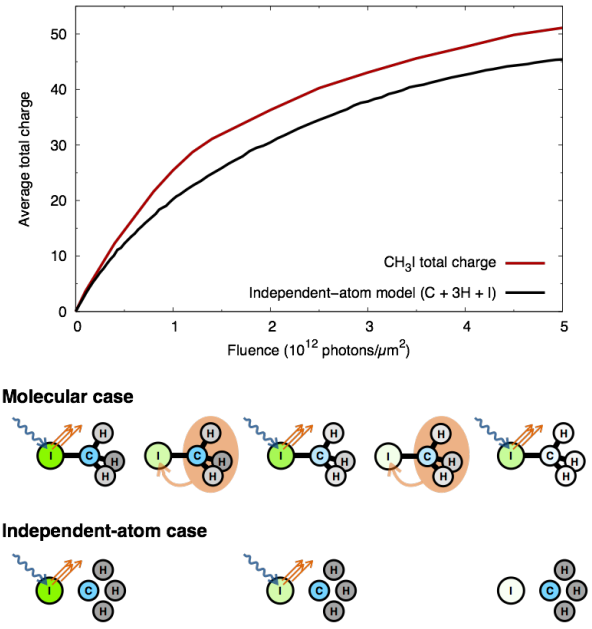

Figure 1. Upper panel: Average total molecular charge as a function of fluence calculated for CH_3I molecules and within the independent-atom model. Lower panel: Illustration of the CREXIM mechanism in the molecular case, in comparison with the independent-atom case.

References

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