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Theoretical study of electronic damage in single particle imaging experiments at XFELs for pulse durations 0.1 - 10 fs by

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Determination of the protein structure is one of the most challenging fields for the modern biological science. X-Ray Free Electron Lasers (XFELs) may allow to single-particle imaging method to employ the determine structure of macromolecules even if the crystalline structure cannot be obtained. Very short pulses (less than 10 fs) allow to outrun Coulomb explosion and minimize radiation damage. However, electronic damage during pulse propagation is still present. Ionization by electron plasma generated in the sample is a major contribution to electronic damage, and it is particularly dependent on the amount of Auger ionization. Since Auger process has characteristic times on the order of femtoseconds, shorter X-ray pulses should decrease its contribution. The effect of electronic damage on the single-particle imaging at pulse durations 0.1 fs - 10 fs and in a large range of fluences was studied to determine the optimal conditions for the single particle imaging experiments.