

Abstract

New generation X-ray free electron laser (XFEL) sources provide novel opportunities for the determination of the structural dynamics of macromolecules. During a high intensity, high energy short duration pulses of XFEL, drastic structural dynamics to the macromolecules occur. So, by using the simulation tool XMDYN, we have studied and analyzed the radiation exposure to the C-60 macromolecule at different energies of the XFEL pulses. Due to ionization, classical Coulomb forces repel each other and hence sample loses its integrity. From the analysis we see that the average charge, average displacement and ionic probability density of the fragments of the C-60 increases with the energy of the laser pulses.