

507th ASRC Seminar

Date: 15:00 ~ 16:00, 14 March

Location: Meeting room 302, ASRC Building

Speaker: Dr. Marie-Françoise Politis

(Université d'Evry, Val d'Essonne)

Title: Fragmentation of 2-deoxy-D-ribose
after K Hole in Oxygen and AUGER
effect: Ab initio molecular dynamics
studies in hydrated phase

In order to reveal the mechanism of radiobiological effects, French and Japanese groups have promoted mutual cooperation on the basis of competitive research funding of JEAE, REIMEI project. Physicochemical process of DNA damage, particularly DNA strand breaks, have been focused as one of the major targets of the project. We have explored the mechanism of DNA strand breaks using *ab initio* molecular dynamics (*ab initio* MD) to reveal early dissociation processes of fragmentation of double ionized deoxyribose molecule in DNA after *K*-shell hole production and succeeding AUGER process. Fragmentation depends on the local environment of the molecule and of the ionized orbital, but maybe not on the position of the *K* Hole. Full electron quantum calculations of most probable channels of AUGER deexcitation has to be done. We are also investigating the reaction of deoxyribose with neighbouring (H₂O) when ionized in O1s orbital. Further the theoretical prospect will be verified by experimentally observing fragment ions from the molecule using synchrotron soft X-rays from Spring-8.

<Contact>

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