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► **To cite this version:**

Damien Tolu, Dominique Guillaumont, Aurélien de la Lande. Simulation of alpha radiolysis in organic phase containing Plutonium at the ultra short time scale. 32nd Miller Conference on Radiation Chemistry, Jun 2023, Furiani, France. cea-04742469

**HAL Id: cea-04742469**

**<https://cea.hal.science/cea-04742469v1>**

Submitted on 17 Oct 2024

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## Simulation of alpha radiolysis in organic phase containing Plutonium at the ultra short time scale

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The PUREX process (Plutonium Uranium Refining by Extraction) is widely used for extracting uranium and plutonium from spent nuclear fuel. It uses liquid-liquid extraction technique with an organic phase made up of tributyl phosphate (TBP) in an organic diluent. During the separation process, the emission of ionizing particles such as alpha particles, resulting from the decay of plutonium, make the organic solvent susceptible to radiolytic, which reduces its performance. The understanding of these phenomena is necessary for the development of new and more radio-resistant extraction processes. It is possible to isolate the degradation products using characterization techniques such as mass spectrometry and to investigate the mechanisms at the short time scale using picosecond pulsed radiolysis. However, the interactions between ionizing particles and extracting molecules at ultra-short time remain poorly known and cannot be studied experimentally.

The objective of this work is to simulate radiolysis event in organic phase containing plutonium and TBP at the attosecond time scale, through numerical simulations using quantum chemistry methods. The simulations are performed using the Real Time Density Functional Theory (RT-TD-DFT) and give access to the charge motions from the electronic dynamics. In order to better understand the effects of an irradiation on an organic molecule, we simulate the energy deposition of a 5 MeV alpha particle on a tributyl phosphate molecule (TBP). The amount of energy deposited varies according to the trajectory and can reach several tens of electronvolts around the impact point. These simulations are performed on free TBP as well as in the presence of plutonium.