

# **Understanding the Interactions between Low Energy Electrons and DNA in Aqueous Solution**

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Ionizing radiation can damage DNA in a cell directly, or it can excite molecules in the cellular surroundings. The Low Energy Electron (LEE) is one of the secondary species produced via this second process. It has been shown that this species can cause significant damage to DNA. In fact electrons with energies as low as 0eV have been shown to cause strand breaks in dry DNA. In the work I will present I discuss the work we have performed to investigate this damage mechanism using a combination of DFT and Molecular Dynamics. At variance with some previous works, in our simulations the interaction between the DNA and the surrounding water molecules are all modelled using DFT. Our results highlight the significant role that water molecules can play in DNA damage reactions and demonstrate that it is therefore important to incorporate explicit water molecules in any simulation of the DNA damage process. In the final part of the talk I will discuss more recent work in which we investigate the reaction between LEEs and a DNA-Cisplatin structure in an explicit water environment.