

Short visit 19/03/2007 – 26/03/2007

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Scientific report

Electron-DNA collision experiments have shown that relatively slow electrons (with energies of about 10eV or less) can lead to the strand breaks in DNA through a mechanism that involves the formation of intermediate resonant states. Therefore, processes that lead to the production of electrons are relevant for the understanding of biological damage. For the study of most of these processes discussed above an appropriate description is required which includes non-Born-Oppenheimer processes. Understanding and handling properly the nonadiabatic dynamics of molecular systems is therefore of fundamental importance.

During the short visit we have chosen particular systems to study in a joint collaboration with the group of Prof. W. Domcke at the Technical University of Munich. As a first step we start the collaboration with the study of the ultrafast photoinduced nonadiabatic processes through conical intersections in pyrazine. Later on making use the experience gained from the treatment of pyrazine we plan to investigate one of the amino acids, the guanine. We had also several discussions with Prof. Domcke and the members of his group concerning the particular details of both the quantum chemical and wave packet calculations.

28/03/2007, Debrecen

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