

Very short lifetimes of excited states of isolated bases in nucleic acids, on the picosecond order, are believed to contribute to photostability of the genetic code. When embedded in DNA this behavior becomes more complex, mainly due to their interactions via stacking and hydrogen bonding. The DNA photophysics is not fully understood yet. It depends e.g. on the conformation and the character of excited states. The studies on smaller systems can help to improve the understanding of these phenomena. The aim of this work was to examine the dynamics of the excited states of the  $n \rightarrow \pi^*$  character of the complex of N-methylformamide dimer and two waters. The study was performed using non-adiabatic dynamics simulations with on-the-fly Surface Hopping algorithm based on the potential energy surfaces and non-adiabatic couplings obtained with multi-reference approach. The results show that after the vertical excitation into delocalized  $S_2$  state the system relaxes into  $S_1$  state within several tens femtoseconds. For majority of the population, the character of the state then oscillates between localized and delocalized during the whole course of the dynamics. Comparison with calculations with the waters removed indicates that the delocalization is caused by waters serving as a bridge between the two chromophores.