Modeling the Electronic Circular Dichroism of DNA and photosensitized DNA

Hugo Gattuso, Xavier Assfeld, Antonio Monari

Université de Lorraine/CNRS, Théorie-Modélisation-Simulation, SRSMC UMR 7565, Vandoeuvre-Lès-Nancy, France

The modeling of DNA photochemistry and its interactions with photosensitizers have recently gained interest because it allows the understanding of DNA photodegradation processes. Moreover photosensitization can be exploited for cancer treatment or simply DNA probing. One of the key aspects that need to be better characterized are the specific modes with whom sensitizers interact with DNA as well as the structural modifications induced in its global structure.

To do so, we studied the electronic circular dichroism (ECD) of two types of B-DNA, the poly(d[AT]) and poly(d[CG]) double strands, with and without photosensitizers and we compared the evolution occurring in the spectra. ECDs were simulated using the Frenkel exciton theory and the conformational space was explored using classical molecular dynamics. Excited states were obtained using QM/MM methods at the TD-DFT level of theory.