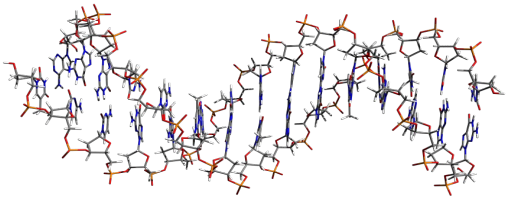
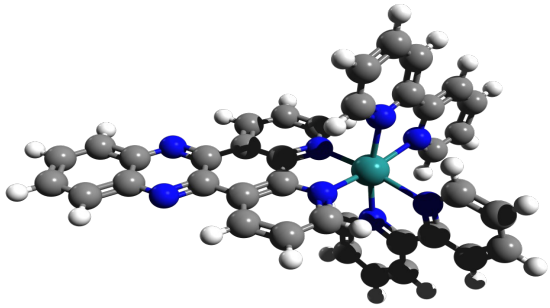
UV-VISIBLE spectra of ruthenium complexes in interaction with DNA

Thibaut Very, Xavier Assfeld

Équipe de Chimie et Biochimie Théoriques (CBT)
UMR 7565 CNRS-UHP
Institut Jean Barriol (FR CNRS 2843)
Faculté des Sciences et Techniques,
BP 70239, Boulevard des Aiguillettes
54506 Vandoeuvre-lès-Nancy (France)





Transition metal complexes are widely used and the coverage of applications is quite broad. In medicine domain, and particularly concerning treatments of diseases like cancer, platinum complex known as cisplatin is given daily. However, the side effects felt while taking this drug are strong. In order to reduce side effects, research has turned toward other transition metal, showing less cytotoxicity, like ruthenium.[1] Combined with polypyridyl ligands, it show interesting photoluminescence properties and can be used as a light probe of the interaction with DNA.

Here we present a combined QM:MM study of the interaction between DNA and a ruthenium complex : [dipyridophenazino,bisbipyridino,ruthenium]$^{2+}$. This complex exhibit fluorescence while interacting with DNA whereas this fluorescence is quenched in aqueous media.[2] Firstly, we carried out MM minimizations on a system made of a 15 base pairs B-DNA, the complex intercalated into the double strand and a cylinder of water molecules, in order to see which configurations are more likely to happen. These calculations are being followed by QM:MM optimizations and finally TDDFT calculations to retrieve UV-Visible absorption spectra. We show the effect of intercalation into DNA for the complex.

[1] Huxham, L.A.,*INORG. CHIM. ACTA.,* **2003,** *352***,** 238-246**.**
[2] Brennaman, M.K. , *J. AM. CHEM. SOC.*, **2002**, *124,* 15094-15098.