Spécialité de Master « Optique, Matière, Paris »

Stage de recherche (4 mois minimum, à partir de début mars)

Proposition de stage (ne pas dépasser 1 page)

Date de la proposition :

Responsable du stage / *internship supervisor*:

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Nom du Laboratoire / *laboratory name*: Institut Galien Paris Sud (UMR CNRS 8612)

Code d'identification : Organisme : Université Paris-Sud

Site Internet / *web site*: www.umr-cnrs8612.u-psud.fr/

Adresse / *address:* Faculté Pharmacie Paris-Sud 5, rue J-B Clément, 92290 Châtenay-Malabry

Lieu du stage / *internship place*: Institut Galien Paris Sud

Titre du stage / *internship title*: Electronic and optical properties of transition metal complexes used as potent anti-cancer photo-sensibilizing drugs

Résumé / *summary*

Context of the study

Photo-chemotherapy is a technique for cancer treatment based on the complementary use of light radiation and a photo-sensibilizing (PS) drug which release its therapeutic effects only under light exposure. After administration to the patient, the drug is absorbed to some extent by the tumor and/or metastases, the cancer tissues are selectively exposed to radiation, which cause cellular damage leading to cancer cell death.

The design of a potent PS is challenging since many criteria must be satisfied. The drug should absorb light within the long-wavelength therapeutic window (red or near IR light) for an optimal penetration of biological tissues, but without being cytotoxic in dark to avoid harming healthy cells.

The transition metal complexes are very promising although their photo-chemistry is still poorly understood in spite of all endeavors. They are particularly interesting notably because of their capacity to absorb visible light more efficiently. Large variety of metals and ligands allows changing the photochemical properties of metal compounds.

Objective

DNA strands are the primary intracellular target of antitumor drugs. A transition metal complex usually intercalates with DNA base pairs or binds with DNA grooves, and this mechanism alters its photochemical properties. To study the binding effect, we propose to perform theoretical calculations on transitional metal complexes to discuss the changes in charge distribution and optical properties of isolated species or embedded in different environments. Fourth-group transitional metal (Cu, Fe,…) complexes with NN-donor heterocyclic ligands will be considered.

Methodology

Density functional theory (DFT) calculations will be done on isolated complexes in vacuum and in implicit solvent using the software Gaussian09. Periodic calculations will be also performed starting from different experimental crystallographic structures and using the software Crystal. Theoretical electron density distributions will be analyzed using proven methods and compared.

Time-dependent DFT method will also be used to access to electronic transitions and optical properties (UV-vis spectra).

Toutes les rubriques ci-dessous doivent obligatoirement être remplies

Ce stage pourra-t-il se prolonger en thèse ? *Possibility of a PhD* **? : YES**

Si oui, financement de thèse envisagé/ *financial support for the PhD***: MENRT**

Lumière, Matière, Interactions		Lasers, Optique, Matière	

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