

MASTER FRONTIERS IN CHEMISTRY

OFFRE DE STAGE DE MASTER / INTERNSHIP OFFER

M2

2021 – 2022

TITRE DU STAGE / INTERNSHIP TITLE:

Modeling the Photo-Absorption Properties of Noble Metal Nanoclusters in Solution

SUJET DU STAGE / INTERNSHIP DESCRIPTION (10-15 LIGNES) :

Noble metal nanoclusters in solution are extensively studied for their impressive spectroscopic properties. They can indeed undergo localized surface plasmon resonance (LSPR). At the metal-dielectric interface, the electrons of the conduction band are able to enter in collective oscillations (plasmon) in response to an applied electromagnetic field leading to extraordinary optical properties.

Although deeply studied at experimental level, LSPR is still at its early stage at theoretical level owing to the size and complexity of the large hybrid organic/inorganic system under investigation. The aim of this internship is to develop a methodology based on Density-Functional Theory (DFT) and its Time-Dependent variant (TD) allowing a comprehensive understanding of LSPR in solution. For that, we will focus on the theoretical investigation, by novel electronic structure approximations, of the environment effects surrounding noble metal nanoclusters in solutions, and we will analyze the impact of these decorations on the resulting surface-enhanced absorption properties.

MOTS-CLÉS / KEY WORDS:

Density-Functional Theory; Noble Metal Nanoclusters; UV/vis Spectroscopy; Plasmonics

DATES ET DURÉE DU STAGE / DATES AND DURATION

February, 7th to July, 22th

CONTACT - RESPONSABLE(S) DE STAGE / SUPERVISOR(S)

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