Report on the outcomes of a Short-Term Scientific Mission[1]

Action number: CA21126

Grantee name: Florent Calvo

Details of the STSM

Title: Sampling the structure and spectroscopy of model asphaltenes

Description of the work carried out during the STSM

Our work aims to build model asphaltene molecules of the continental type and to examine their physical chemical properties, with a focus on infrared spectra. In this STSM we have extended a simple computational tool to generate such molecules stochastically, by surrounding a central aromatic domain with randomly distributed and generated aliphatic side chains.

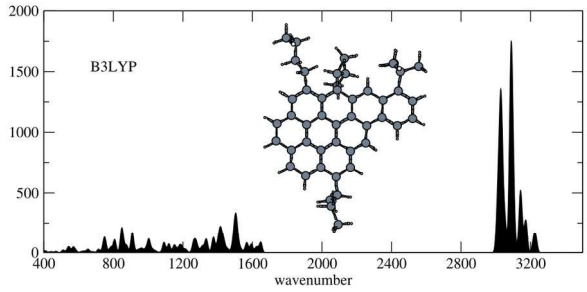
During the visit, we tested the stochastic generator under broad conditions of size, H/C ratio, nature of the aliphatic chain (elongated vs branched), and produced limited databases, for model asphaltenes of the 'continental' type. The purpose of the collaboration is to benefit from the expertise of the spanish partner in quantum chemistry, so we also tried to determine IR absorption spectra for small molecules thus generated in the first part.

This was achieved using density-functional theory, using a reasonable but efficient functional (B3LYP) together with a good correlation-corrected basis set.

Description of the STSM main achievements and planned follow-up activities

We have verified the robustness of our stochastic generation method, and the ability to generate realistic molecules that satisfy prescribed stoichiometries (H/C ratio) and external geometric parameters that influence the shape of the central aromatic domain or the type of aliphatic side chains. The DFT calculations of the IR absorption spectrum are promising, and we illustrate below our first result obtained for a small model asphaltene molecule of about 30 carbon atoms.

[1] This report is submitted by the grantee to the Action MC for approval and for claiming payment of the awarded grant. The Grant Awarding Coordinator coordinates the evaluation of this report on behalf of the Action MC and instructs the Grant Holder Manager to verify the grant documents compliance and proceed with the payment.



The planned activities will be

-to generate reduced databases of model asphaltenes of comparable size (<50 atoms in total) but with varied morphological attributes, to be processed at quantum chemical level

-to use the DFT data to parametrize a machine learning model to predict IR absorption spectra

-to generate more extended databases for model asphaltenes that are hardly tractable by quantum chemistry

-apply the ML model to these extended databases

-analyse the structural and spectra data using classification tools, possibly using unsupervised machine learning.