Project PN-III-P4-ID-PCE-2020-2783
scientific summary

The present project had 4 objectives scheduled for 2021. All of them have been achieved.

1) Update the computer cluster at ULBS

In April 2021 two additional servers and two 16 TB SSD hard disks have been added to the computer cluster at ULBS.

2) Start the computation of VCD spectra

From May till November 2021 we (i.e., Dr. Dragos Isac and Dr. Paul Nicu) have computed VCD spectra for 13 very flexible chiral molecule. Approximately 15k molecular conformations have been computed at DFT level of theory.

3) Start machine learning techniques for analysing VCD spectra

Under my supervision, Mr. Gabriel Marton has developed a Python code that uses machine learning (ML) algorithms to identify the VCD general coupled oscillator fragments. We have considered four different clustering algorithms, i.e., K-means, Spectra, Agglomerative and NSGA-III. Currently, we are fine tuning the fitness functions used by the NSGA-III algorithm, which so far has yielded the best results.

4) Develop a website of the data based where VCD spectroscopists can upload their experimental spectra.

A working version of the website, which allows one to upload experimental data (up to 25 MB), can be found here **here**.

In addition, I was involved in two collaborations, one with Dr. Wybren Jan Buma (University of Amsterdam, Netherlands) and one with Dr. Thomas Bürgi (University of Geneva, Switzerland). These collaborations have resulted in two papers.

Valentin Paul Nicu
December 10, 2021