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

Action number: CA21126

Grantee name: Ransel Barzaga Guzmán

Details of the STSM

Title: Predicting the infrared emission of carbonaceous materials: A combined DFPT-BEC and ML approach

Start and end date: 10/03/2024 to 21/10/2024

Description of the work carried out during the STSM

During this STSM, Dr. Ransel Barzaga visited the Department of Chemistry, Aalto University; concretely to the group under the leadership of Dr. Miguel Caro and that also has the expertise of Dr. Rina Ibragimova. In this sense, this group has specialized in the development of Machine Learning (ML) potentials to the design of amorphous carbon materials using molecular dynamics. The goal of the visit was to establish the ground basis for the development of ML potentials focus on hydrogenated amorphous carbon (HAC) materials. Firstly, standard calculations were performed to get knowledge of the principles behind the TURBOGAP code, which will be the one used for the simulations. Different simulations of molecular dynamics were carried to describe the evolution of carbon materials from pure amorphous to graphitize ones. According to the tests at several temperature range, seemingly, should be appropriate to use metastable states from the molecular dynamics calculations in order to get a set of structures, which are produced at different ramps of temperature as in the astrophysical conditions. Concerning the infrared emission (IR) of these HAC materials, which was another of the objectives of the STSM, the main route so far distinguish in order to tackle this problem was, firstly, to distinguish if it is possible to compute the infrared intensity through the Perturbation Theory of Green functions instead of the Density Functional Perturbation Theory. The final goal in this case is to obtain, in principle, more accurate infrared intensity, which can be applied to train in the future an IR-ML potential. Another bottleneck identified during the STSM visit is the selection of the benchmarking database needed to set the training for the future ML potential. A mixture of molecules were selected according to previous databases used to build potentials for similar materials, although, this process requires further adjustments.

[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 GH for payment of the Grant.

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

The main achievements of the STSM were the identification of some metastable states during the performance of molecular dynamics calculations, which could have an astrophysical interest. Specially, because the structures from these metastable states can evolve to different materials, contrary, to the typical evolution of amorphous carbon to graphite. The new materials were a combination of amorphous carbon and graphite fragments which probably will transform into more complex systems once the ML potentials of CH are developed. In fact, we expect that under the inclusion of hydrogen atoms in the molecular dynamics simulations the diversity of metastable states increases giving rise to HAC materials with some structural peculiarities. Another achievement from the STSM is the identification of a more automatic way to extract fragments of larger models. Particularly, extracting those fragment from models composed of 500-1000 atoms to compute the IR spectra but using only 200-500 atoms. The identified approach was the Special Quasirandom Structures method, which allows the extraction of the fragments retaining the chemical environment produced by the PBC conditions. This will minimize the needed time for the following reoptimization of the fragments, something mandatory before performing the IR spectra calculations. The planned activities towards future collaborations imply a benchmarking of the CH potential applied to the HAC materials that eventually will be produced in the molecular dynamics. A profound analysis of the aromaticity of these HAC materials (Csp2/Csp3 ratio) in order to distinguish any anomaly in the performance of the ML potential. In addition, the production of several metastable states that can produce extreme structures either for their morphology or for the level of hydrogenation. Another key point is to perform the simulations of the hydrogen bombardment of the new HAC materials but applying the slab model, for which the thickness has to be also determined. Finally, the design of the IR-ML potential has proven to be a complex task that requires more work on the fundaments. Particularly, concerning the way they can be implemented since vectorial properties, like IR emission, are more difficult to include in the training of the IR-ML potential. Thus, it has been identified the need for a second visit to the Chemistry Department, Aalto Univeristy; this time for a longer period of time, in order to carry out the first steps in the implementation and fundaments of IR-ML potential.

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