VIRTUAL MOBILITY (VM) GRANT
REPORT TEMPLATE

This report is submitted by the VM grantee to VNS Manager, who will coordinate the approval on behalf of the Action MC.

Action number: CA18222

VM grant title: Potential of ultrafast electron diffraction to study the correlated electronic and nuclear motion in Uracil:Numerical Simulation

VM grant start and end date: 15/09/2021 **to** 13/10/2021

Grantee name: Purbaj Pant

Description of the outcomes and achieved outputs (including any specific Action objective and deliverables, or publications resulting from the Virtual Mobility).

(max. 500 words)

Within the Virtual Mobility program, we have proposed to conduct a numerical simulation to understand the usefulness of the ultrafast electron diffraction in understanding the correlation between the ultrafast electronic and nuclear correlation in the photo-excited nucleobases.The project was highly ambitious to be completed withtin a time period of a month. But, important in roads has been made standing on which the future developments can be made.

Within the grant period we have developed in-house code to compute the the ab-initio elastic and inelastic lectron escattering from a molecule. Unlike the tradiation independent atom model (IAM), the ab-initio model includes contribution from both the nucler wave function and the electronic wave function (also valence electrons) while computing the scattering signal. Hence, in the calculated diffraction pattern represents the sum of both the ineleatic and elastic scattering signal. Such calculations offers the grounds to further study the correlated electron and nuclear dynamics, imaging of conical intersection in the nucleobases and electron and protron tunnel in other organic molecules.

For current studies, we have used Uracil as the model system. From literature it is understood that the photo-excited uracil shows correlated electron and nuclear dynamics at ultrafast timescales. In order to probe the problem we started with the calculation of static scattering signal. The electronic structres and the molecular orbitals necessary for the computation of the diffraction was generated by performing ab-initio calculations at the level of CASSCF(2,2) level of theory using the def2-SVP/C basis.The molecular orbital density matrix thus obtained from the calculation was used to obtain the diffraction pattern. The diagonal components of the matrix was used to compute the elastic scattering and the non-diagonol componenets were used to compute the inelastic scattering. To make a comparision, we have also calculated the diffraction pattern using

IAM model. Form the calaulations, it is obvious that there is a significant contribution of the electronic wavefunction in the scattering pattern. Standing on these calauclation further study on the correlated electornic and nuclear dynamics in uracil shall be made.

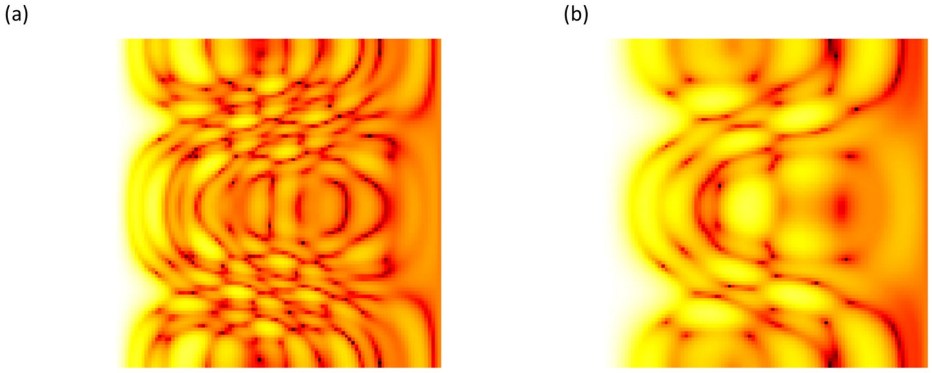

Figure 1 The diffraction of uracil calculated by (a) ab-initio method and (b) by using the independent atom model

Description of the benefits to the COST Action Strategy (what and how).

(max. 500 words)

The cost action focuses in the development and dissemination of the knowledge in the ultrafast processes in the chemistry. One of the less understood phenomnenon in the ultrafast chemistry is the fine-stroke picture of the correlation of the nuclear and electronic dynamics in photo-excited molecules (systems).The project aims at the development of a framework where such phenomenon can be extensively studied.Such an effort would be beneficial to the fellow workers in the cost Action.We have paved an in-roads to make such framework. Thus the simulation performed during this grant-period can later be useful to meet the broader targets of the cost action.

One of the objectives of the cost action is to translate the cutting edge research from the scientifically advanced countries to the ICT countries and promote the involvement of the Early carrrer invesitgators in leading such translation. There are very few groups in ICTs working on ultrafast structural studies of photo-excited system.This project has been completely run by an ECI in an ICT nation. Such efforts in furture can promote the use of ultrafast X-ray and electron diffraction in studying the dynamics in photo-excited systems.This perfectly aligns with the philosophy of the cost action.

This project has been a beginning of the collaborative efforts between researcher in Poland and the Czech Republic. Through this project such collaboration shall be extended by seeking additional funding opportunities. Such efforts are always beneficial to the cost action.

The project aims to develop a simulation platform to support the experimental effort in understanding the electronic and nuclear dynamics in molecules.The cost action has a special workpackage to develop such efforts. The grantee, with the experience from the current studies, in future can contribute in the activities of the workpackage.

Description of the virtual collaboration (including constructive reflection on activities undertaken, identified successful practices and lessons learned).

(max.500 words)

The virtual mobility grant has been a huge support in the pandemic era to eastablish the collaborating efforts. Through this grant I have managed to initiate a collaboration in a completely new domain of research, which is far from my previous experiences and

academic trainings.

During the grant period, i have worked very closely with my collaborators. Sharing of resources and ideas has been done on frequent basis. We have conducted weekly online meeting to motior the progress of the project. The collaborators have shared their expertise and the knowledge to push the project forward.The virtual collaboration has supported the project immensely.

Of the various efforts, making an online discussion channel through paltform like SLACK has been very productive and beneficial. Regular online meetings with the collaborators has been quite helpful. Identification of problems and solution has been very effective.

From the experience i have gained during the grant period, virtual collaboration is an efficient alternative to the traditional collaborative efforts. At times, for pojects concerned with the development of simulation system, virtual collaboration can be even more efficient than the traditional method of collaboration. Sharing of file systems, the input files for the softwares, was very effieicient during the virtual collaboration. Also, a common code-writing, edtiting was performed through the Jupitier notebook which paced the efforts substantially.

In overall, for me, the virtual collaboration was extremely helpful and I plan to keep the collaboration ongoing by securing additional funding through various means.