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 Action (AttoChem)

VM grant title: CApturing satellite states in the Photoelectron Spectrum (CAPS)

VM grant start and end date: 07/09/2021 **to** 12/10/2021

Grantee name: Torsha Moitra

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

The project has been successfully completed by fulfilling all the objectives in the proposal. A strategy to compute accurately the high energy region of the photoelectron spectrum, characterised by low intensity features has been established employing equation of motion coupled cluster singles doubles and perturbative triples Dyson orbitals. The correlated Dyson orbital description of the bound part was coupled to multi-centric B-spline time dependent density functional theory continuum orbitals, to compute individual channel photoionization observables. The general strategy developed is applicable for both valence and core ionizations. During this period a manuscript detailing the theory and results has been prepared and submitted, titled "Multi-electron excitation contributions towards primary and satellite states in the photoelectron spectrum." (10.33774/chemrxiv-2021-g0ktd)

The work directly contributes to the aim of working group 2, by developing new theoretical technique for the description of ionization in molecules.

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

One of the primary goals of the COST Action Attochem is to foster theoretical efforts to study attosecond processes, photoionization being a dominant process as attosecond pulses have photon energies far exceeding the ionization threshold of most molecules. Here, we have developed a highly correlated approach for studying photoionization processes by combining coupled cluster Dyson orbital description with multi-centric B-spline TD-DFT continuum orbitals. The developed method has been validated for molecular systems and has been shown to reproduce complex experimental observations like Cooper minima, shape resonances and autoionization resonances, for instance.

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

The project lead to a fruitful collaboration between Prof. Piero Decleva (UNITS, Italy), Prof. Sonia Coriani (DTU, Denmark) and the applicant - Torsha Moitra (DTU, Denmark). The completion of the project was brought about by exploiting the expertise of the applicant and the collaborators. Prof. Piero Decleva's Tiresia program was used for the computation of the continuum orbitals and subsequently the observables. Prof. Sonia Coriani helped understand the nature of Dyson orbitals generated and analyse the photoelectron spectrum obtained with the hierachy of coupled cluster method (CCSD and CC3). Torsha Moitra interfaced the EOM-CC3 Dyson orbital coefficients obtained from e^T program with Tiresia code, carried out the calculations and wrote the first draft of the manuscript. All authors revised the manuscript before submission.

The work was accomplished by weekly online Zoom meetings. In the meetings, plans were made and results were discussed. The computations were carried out on DTU HPC. T.M, S.C and P.D have accounts on DTU HPC, and were allowed to read/write in each others directory. This enabled all the participants to follow the progress of the work closely. Further analysis and post-processing results were shared via email. The manuscript was prepared and editted using the free version of online latex tool - Overleaf.