SHORT TERM SCIENTIFIC MISSION (STSM)
SCIENTIFIC REPORT

This report is submitted for approval by the STSM applicant to the STSM coordinator

Action number: CA18222
STSM title: Development of theoretical methodologies for the description and interpretation of time-resolved spectroscopic and scattering experiments in the femto- and attosecond time scale
STSM start and end date: 30/08/2021 to 15/10/2021
Grantee name: Anna Kristina Schnack-Petersen

PURPOSE OF THE STSM:

(max.200 words)

In a collaboration with the group of Prof. Henrik Koch at NTNU, I aimed to implement an efficient Cholesky based code for determining both ground and excited state geometrical gradients at the CCSD level of theory in the open source program eT. These gradients are not only required for performing geometry optimizations, they are also essential for simulations of nuclear dynamics. In order achieve this efficient implementation the code was to be thoroughly tested to avoid bugs and in order to ensure its efficiency the bottlenecks of the code was to be identified and optimized. In addition, we would begin to compare the new implementation to both commercial implementations as well as older implementations in open source programs, where the gradients are available. Furthermore, a geometry optimization algorithm was to be implemented in the program in order to allow for geometry optimizations of both ground and excited states.

If time permitted I would also work on developing methods for performing resonant inelastic X-ray scattering (RIXS) calculations also at the CCSD level of theory. Once again the code was to be optimized and calculations performed in order to compare both to other implementations and to experimental data.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

(max.500 words)

Gradient project:

The code for the gradient is now optimized to a satisfactory degree and all bugs have been fixed. Thus, gradients for both the ground state and excited state are available at the CCSD level of theory. We have begun the process cleaning up the code. For this purpose, the code has been split in three parts and the first (an F-transformation) has been cleaned up and is now available in the master branch of the code. The second part to be cleaned up is the geometry optimizer. This has been generalized in order to be usable both at the HF (gradients already available) as well as the CC level of theory. This part has not yet been finally approved for adding to the main branch, but work continues. The final part of the code to be cleaned up is also the main part, however as it depends on the other two, the final clean up cannot take place until the other parts are approved.

Benchmark calculations are being carried out for 3 test systems at the ground and excited state with our code as well as in QChem and Psi4 (here only for the ground state), in order to test the efficiency of our implementation.

A first draft for the introduction as well as the theory for the article presenting the gradient

implementation has also been written.

RIXS project:
The code clean-up for better readability and efficiency has commenced, but is not yet finished. Calculations for testing the code have also begun.

DESCRIPTION OF THE MAIN RESULTS OBTAINED
(max 500 words)

A Cholesky based gradient code has been developed for an open source program, and is expected to improve efficiency over other non-Cholesky based implementations. In addition, both ground and excited state gradients are available and thus geometry optimizations at the CCSD level can be performed at both ground and excited states. Furthermore, the availability of the gradients is the first step towards excited state nuclear dynamics at CCSD level, and thus we are one step closer to achieving this.

FUTURE COLLABORATIONS (if applicable)
An article about the gradient code is in preparation and further testing of the code will take place. In addition work continues on the RIXS code