Excited States and Nonadiabatic Dynamics CyberTraining Workshop 2021

Work Report

I am Sunita Sharma, a 3rd year Ph.D. student working under the supervision of Prof. Gopalan Rajaraman, in the Department of Chemistry, IIT Bombay, India. I have been working on Molecular Modelling of metal-mediated catalytic reactions. I mainly use Gaussian and ORCA software for my work. I have attended this workshop "**Excited States and Nonadiabatic Dynamics CyberTraining Workshop 2021".**

Experience-

It was a truly great experience while I have attended this workshop. Learned so many software's and how can I use this software's in my research work. I have gained little bit experience of python language, libra software, CP2k calculations, NEXMD calculations, coulombs software. I have tried to apply NEXMD and CP2K for my project of this workshop.

My Workshop Project-

Transition metal complexes play an important role in chemical reactivity. Recently, the light-induced reactivity (photocatalysis) of these transition metal complexes gain interest due to enhance reactivity with the involvement of excited states. For this workshop I have tried to do a theoretical study of Ferric oxalate photolysis (ACS Earth Space Chem. 2017, 1, 5, 270–276). Here, Fe(III) oxalate, $Fe^{3+}(C_2O_4)_3^{3-}$ as an active photo metal complex shows the production of CO_2 via intramolecular electron transfer reaction. So during the reaction Fe(II) oxalate changes to Fe (III) and later it followed by the cleavage of Fe -O bond and CO_2 will release. So, studying the reactivity for both excited state and ground state would be really interesting for the photochemistry branch.

$$Fe^{III}(C_2O_4)_3^{3-} \xrightarrow{h\nu} 2Fe^{II}(C_2O_4)_2^{2-} + 2CO_2 + C_2O_4^{2-}$$

What I have learned in Workshop-

During the workshop I have gone through the 12 days tutorial workshop. In day first tutorial I learned about python and have tried to write Runge Kutta 4th order code by own, also have got the idea of git-hub. In another workshop I have tried to do CP2K calculations in qmflow workshop. Where I have done tutorial of ethylene molecule and for my project I have tried to do CP2K calculations for ferric oxalate (By changing the active space, but I think some basis set error I was getting, so it has not worked out). In another tutorials I have tried to do NEXMD for ethylene molecule (from learning purpose). I have tried to do it for my Iron Oxalate, but there was some error for Iron atom was coming. So, I have fulfilled all tutorial with ethylene molecule. I have also leaned about EOM, beautiful lecture it was. And from many lectures I got knowledge of surface hopping, that was a really different and interesting field I have found apart from my research work.

So, I would like to say that doing all tutorial parts with the instructors was really a fun. I leaned a lot. But need to explore more.

Acknowledgment-

I would like to thank all the Instructors and organizers of this workshop. I want to express my sincere gratitude to “Prof. Alexey Akimov” for giving me a chance to explore the excited state chemistry on a different level. It was really a great experience working with highly knowledgeable persons.

Thank You.