

## **Report for Cyber-training workshop**

In the cyber training workshop, I have learnt and explored a lot of computational tools that were quite new for me. I even haven't used jupyter platform before this workshop and now I can use it confidently. Beside this, I tried to follow all the tutorial sessions, and found the NEXMD software to be most suitable for the project that I proposed to get done during the abstract submission. I actually wanted to simulate the molecular dynamics of cytosine molecule in the excited state, which I wanted to do with Newton-X. But I realised I need to learn more about the software (though I could follow the tutorial, but it seemed a bit complicated to give input in that). So, I have done a few calculations with NEXMD. Following the tutorial, I could do a single point calculation of the molecule in the ground as well as excited state. Also, the geometry optimization in both the states are also done. I have done dynamics in the ground state without any friction though it needs to be done with friction but should require an accurate spectral density. This needs to be figured out from literature, but I don't have enough information about it right now. I could not give the project a perfect shape, but at least I was able to learn about tool, how the excited state dynamics can be simulated using NEXMD. Before that I have done surface hopping only for model systems using my own codes.

At last I want to say that it was a great opportunity for me to learn tools that I have never seen before. I want to express my sincere gratitude to all the instructors and organisers for it.