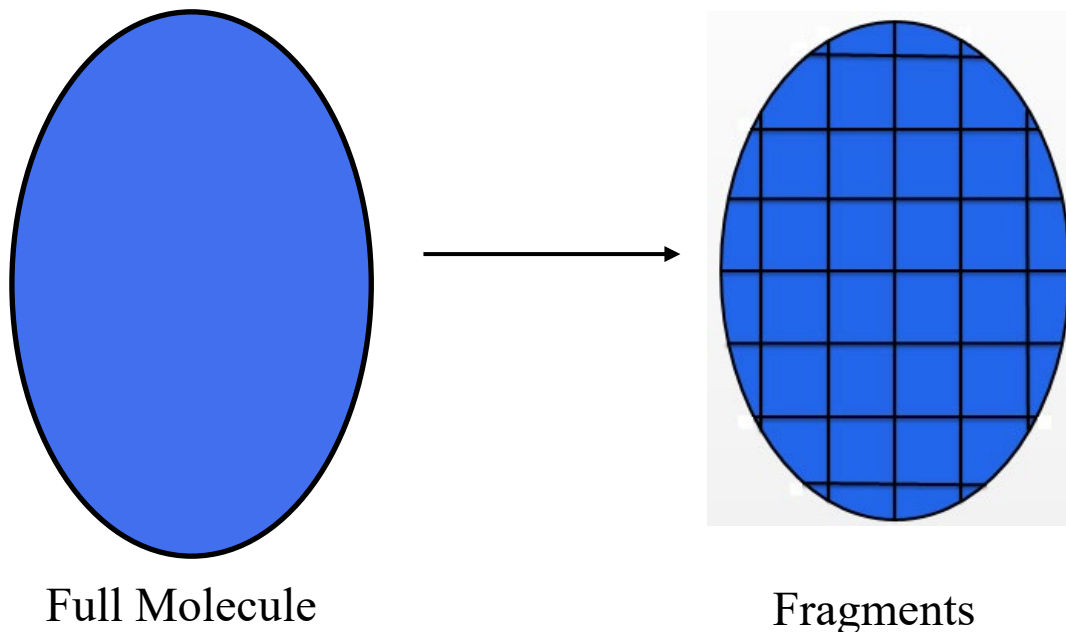

Sibali Debnath

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- Accurate QM and MD simulations to understand the fundamental interactions in supramolecular systems
- Fragmentation based approach for treating large molecules using accurate QM methods



- MD simulations to investigate the conformational space of complex molecules

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Challenges

- Post-trajectory analysis : Accelerating the analysis of output trajectories
- Visualizing complex (high dimensional) data

Things I want accomplish in the summer institute

- How python can be used for HPC ?
- Different techniques to visualize the scientific data
- Learn about GPU computing and programming