Spectroscopy of molecules in their biological environment

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Spectroscopy refers to studies of light–matter interactions and is used to probe molecular and electronic structures of complex systems in nanotechnology and life sciences. Theoretical computer simulations, or *electronic spectroscopy*, must accurately describe the temperature-driven molecular dynamics (MD) as well as the electromagnetic-field-driven electron dynamics (ED). In photophysical applications, it is often reasonable to treat the former with classical force field MD and the latter with quantum mechanical (QM) response theory approaches.

In this presentation, I will illustrate this combined approach to two case study:

- The electronic circular dichroism of DNA and fluorescent stain attached to it.
- The absoprtion and fluorescence of probes used for amyloid fibrils that are pathological hallmarks of a number of human neurodegenerative diseases such as Alzheimer's and Parkinson's.

To help in the identification of the potential adsorption site, we have developed within SeRC and in combination with the visualization center (Norrköping), a visual exploration software tailored for large-scale spatio-temporal molecular dynamics simulation data. The identification of interaction "hotspots" is achieved with use of combined filter parameters connected with probe molecular planarity and probe-fibril interaction energetics.

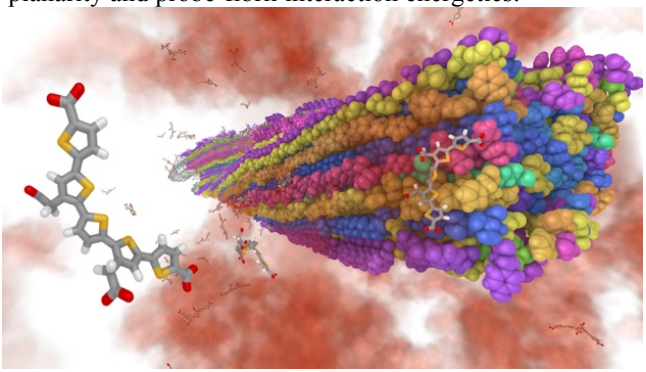

Figure: The probe movement can be observed from the red density field, depicting their spatial distribution integrated over time. The rendering above is produced by the presented visual exploration environment, which enable query driven exploration of spatio-temporal molecular dynamics simulations.