Aggregation Dynamics and Optical Properties of L-Lysine in Aqueous Solutions: a combined MD simulations and experimental study

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L-lysine, an essential amino acid, exhibits intriguing optical properties in aqueous solutions that have yet to fully elucidate. Despite its crystalline form lacking emission, L-lysine emits blue light in aqueous solutions as the concentration increases. These optical properties cannot be attributed to structural features such as the presence of aromatic species or conjugated bonds. This talk will focus on understanding how aggregation affects these optical phenomena. While the zwitterionic nature of amino acids at their natural isoelectric point could suggest that the aggregates responsible for the optical properties are formed through ionic interactions and hydrogen bonds, TD-DFT calculations of UV absorption do not support this hypothesis. [1] Due to the flexible nature of L-lysine, sampling the aggregates formed in aqueous solution at various concentrations is not a trivial task. In this talk, I will discuss how molecular dynamics simulation trajectories of model systems (see Figure 1) can be analysed to gain insight into the structure of the aggregates (see Figure 2) and describe some limitations of the method. [2,3]

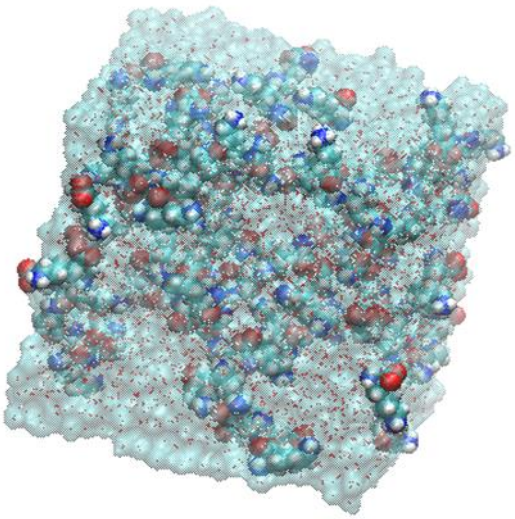

Figure 1 – Example of simulation box of an aqueous solution of lysine 1M.

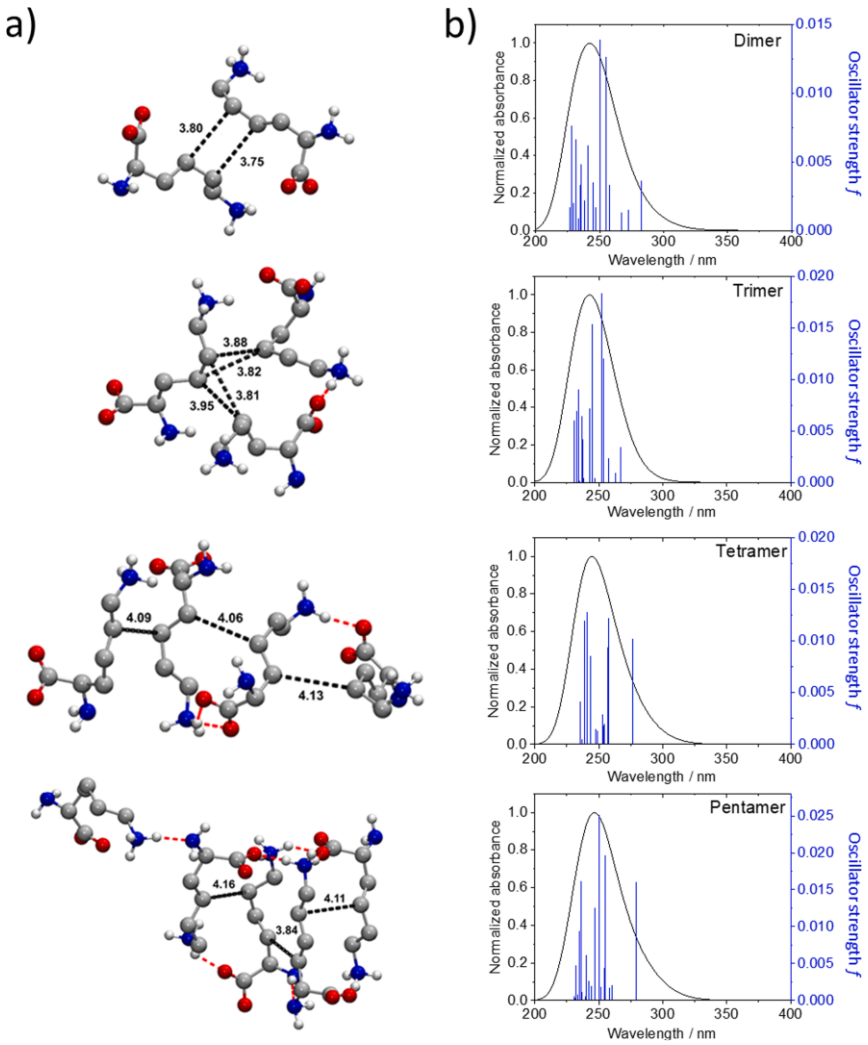

Figure 2 – Examples of hydrophobic associations in lysine aggregates observed in MD simulations of lysine's aqueous solution.

REFERENCES

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