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Self-Assembly of non-covalently bonded hydrogels investigated using Molecular dynamics simulations

N. M. Froböse

FU Berlin, Arnimalle 22 14195, nikolasmif98@zedat.fu-berlin.de

I apply for a poster, in which I want to present my results and experience I gained during my first year in molecular dynamics simulation research and beginning of my PhD:

Hydrogels, with their unique physiochemical properties and versatile applications have emerged as promising materials in various fields, ranging from biomedicine to soft-matter robotics and sensors. Understanding the molecular mechanisms on the atomic level governing their behaviour is crucial for optimizing and rationalizing their functionality and design.
However, atomistic resolved structures of self-assembled hydrogels remain unknown, due to limitations of experimental approaches. Molecular dynamics simulations (MD) however, is a theoretical method that can resolve dynamic processes up to the atomistic level.
In the study I would like to present, we conduct a comprehensive investigation into the viscoelastic properties of self-organized hydrogel structures and dynamics at the atomic level using advanced molecular MD techniques to explore the knowledge gap between macroscopic properties and atomistic structures. Additionally, we present a benchmark assessing the stability of non-biased MD simulation and the determination of viscosities in Newtonian liquid systems namely methane, water, ethane and glycerol.
Our results demonstrate how viscosity estimations are feasible and self-assembly contributes to the physio-chemical properties of a gel, leading to a step towards the rationalization of hydrogel design.
The obtained results provide a summary to conduct a stable NVE simulation for any MD system and useful insights for rationalising physio-chemical characteristics of self-assembled hydrogel peptides and their structural formation and stabilization