



Polymers under Multiple Constraints

Polymer- & Soft-Matter-Seminar

Tuesday,
6th November
2018

Dr. Samuli Ollila

(Institute of Biotechnology, University of Helsinki, Finland)

at: 5.15pm

“Combining MD simulations and NMR experiments of lipid bilayers and proteins”

VDP 4 1.27,
Von-Danckelmann-Platz 4,
06120 Halle

Direct comparison between MD simulations and NMR experiments can be used to interpret the experiments and improve simulation models. This has been especially useful for the studies of ion binding to lipid bilayers, oxidized lipids and disordered proteins. I will present improvement and validation of MD simulations models for lipids and proteins together with the interpretation of order parameters measured from solid state NMR and spin relaxation times measured from solution state NMR.



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