Entanglements of Topological Polymers

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I will talk about computational investigation of dense polymeric systems where the topology of the polymer chains determines the system's conformational and dynamic properties. With the example of a nonconcatenated ring polymer melt I will illustrate how we find and quantify the relevant geometrical and topological constraints in these systems using a combination of minimal surfaces, topological invariants and network analysis [1,2,3]. Using externally driven (or active) blocks on the polymers, we can shift the prevalence of certain entanglements to alter the dynamic properties and generate a novel type of glass. This 'Active Topological Glass' [4] differs from ordinary polymeric glasses as i) it occurs at constant density and temperature, ii) the monomers are not caged by their neighbours and iii) the glass transition results from the topology of the chains.

[1] J. Smrek, A. Y. Grosberg, ACS MacroLetters (2016)
[2] J. Smrek, K. Kremer, A. Rosa, ACS MacroLetters (2019)
[3] C. Micheletti, I. Chubak, E. Orlandini, J. Smrek, in preparation (2022).
[4] J. Smrek, I. Chubak, C. N. Likos, K. Kremer, Nat. Commun. (2020)