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Origins of polysaccharide conformation and viscoelasticity in miscible heterogeneous solvent

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Polysaccharide polymers constitute the fundamental building blocks of life and display a diverse set of conformations resulting in complex viscoelastic behaviour in their solutions; the origins of which need further understanding. Utilising a model high molecular weight, high Trouton ratio 'pectin' polysaccharide extracted from okra (Abelmoschus esculentus) mucilage, we combine computational (molecular modelling and dynamics simulation) and experimental (rheology, calorimetry, and small-angle scattering) investigations, to unveil the underlying microscopic hydrodynamic origins of polysaccharide conformation. In miscible heterogenous solvents of water and glycerol, we observe that the polysaccharide chain undergoes a non-monotonic conformational transition from flexible-to-swelled-to-collapsed configurations, resulting in pronounced viscoelastic responses. The conformational transition is entropy-driven. Although Kirkwood-Buff integrals and preferential binding coefficients indicate preferential exclusion being more significant for water compared to glycerol, molecularly adsorbed water molecules within ca. 0.40 nm of the chain surface have increased 'residence time' with an increase of glycerol in the solvent composition. We postulate that this increased water residence elicits an entropically unfavourable dynamic solvent heterogeneity, which is ameliorated by swelling and collapse of polysaccharide chains. Our results offer new fundamental insights which were previously inaccessible through mean-field assumptions.

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Sitzung Einordnung: Mounting Posters, Beer and light Dinner

Track Klassifizierung: Soft Matter