Summer School on Polymeric Networks for Sustainable Development

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Computational Rheology of Vitrimers – Linking Molecular Dynamics to Macroscopic Flow

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This lecture introduces the fundamentals of vitrimer rheology from a computational perspective, focusing on how molecular dynamics (MD) simulations can be used to understand and predict the mechanical response of vitrimers.

We will begin with a brief overview of vitrimer chemistry and their dynamic covalent bond networks, followed by an introduction to coarse-grained MD techniques tailored to capture bond exchange reactions and network evolution.

The main focus will be on how stress relaxation, viscosity, and viscoelastic moduli emerge from molecular-level processes.

We will discuss how to simulate and interpret linear and nonlinear rheological behavior (e.g., shear thinning, stress overshoot), and highlight connections to experimental rheology.

We will introduce concepts from microrheology and show how tracer-based simulations can probe local viscoelastic heterogeneity.

The lecture will emphasize the unique challenges and opportunities in simulating adaptive polymer networks like vitrimers and how these simulations can support material design.