

Complex Fluids Theory and Simulations

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Summary

- We use [theory and simulations](#) to relate microscopic dynamics and structure of complex fluids to their macroscopic properties.
- We [collaborate with experimentalists](#) to address mechanisms of phenomena that occur on nano to micro-scale and create tools to predict soft matter behavior.
- The complex fluids that we are interested are transient networks, nanocomposites, and jammed suspensions.

Tools for our projects

- Theory:

- Polymer physics
- Fluid mechanics
- Solid mechanics
- Scaling methods

- Simulations:

- Molecular dynamics
- Monte Carlo
- Discrete particle
- Continuum mechanics

I. NRT-HDR: Graduate traineeship on advances in materials science using machine learning



Goals:

- Discover materials with AI
- Skilled in digital data, AI, ML
- Effective team member in diverse group
- Work in multi-disciplinary setting

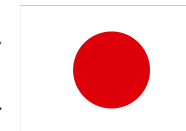
Research topics:

- Additive manufacturing of polymeric composites
- Batteries and solid-state polyelectrolytes
- Sustainable and recyclable polymers
- Tuning data management and machine learning tools

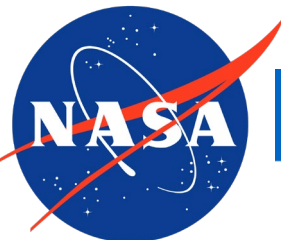
Lab rotation:

Collaborators: Profs. Jana, Wang, Duan, Tan, and Cheng

International partners: Germany , South Korea, Japan



External collaborators: AFRL, NASA, Eaton Corporation, Goodyear, Bridgestone



II. Micro-dynamics and macroscopic flow of soft solids

Personal care products



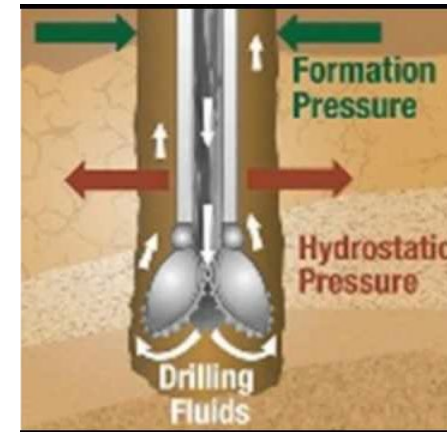
Delivering coatings to paper



3D printing

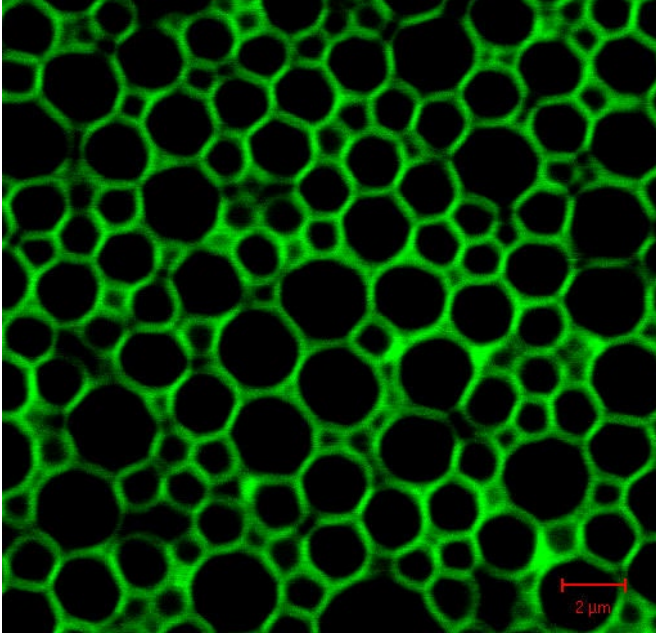


Drilling mud

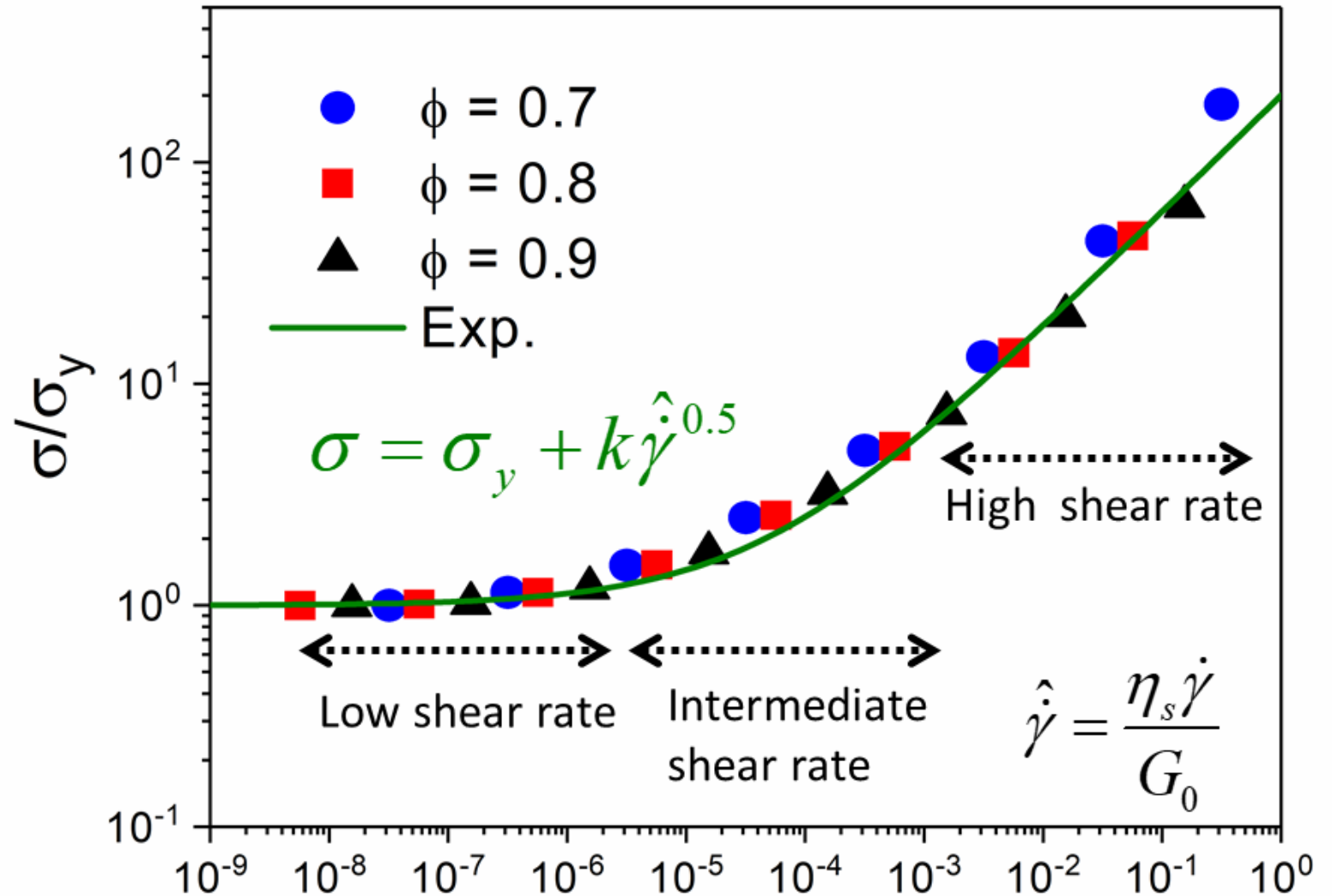


- More than 10,000 tons for formulation applications
- Drilling fluid market: 1.07 Billion USD in 2017

II. Current understanding

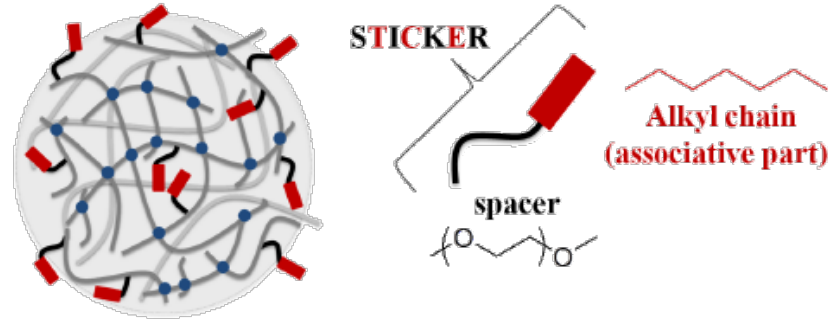


Khabaz et al. Phys. Rev. Fluids., 2017.
 Khabaz et al. Phys. Rev. Fluids., 2018.
 Liu et al. Soft Matter., 2018.
 Khabaz et al. J. Rheol., 2020.
 Bonnecaze et al. J. Rheol., 2020.
 Khabaz et al. J. Rheol., 2021.
 Liu et al. J. Rheol., 2021.
 Khabaz and Bonnecaze, Phys. Fluids, 2021.
 Di Dio et al. J. Rheol., 2022.



II. Micro-dynamics and macroscopic flow of soft solids

New microgels!



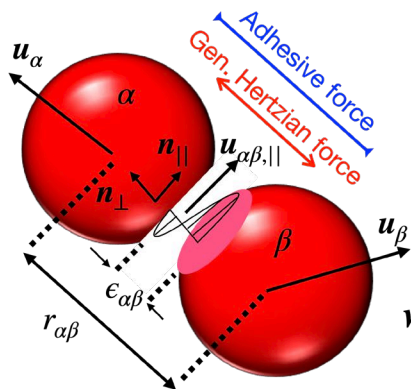
Key factors

- Adhesive forces
- Flow strength
- Residual stress
- Boundaries

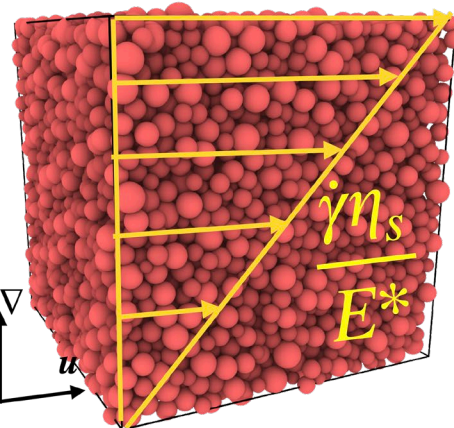
Objectives

- Predict flow curves
- Characterize role of residual stress on transient rheology
- Identify mechanism of DHs and plastic deformation
- Use trajectories to design an ML model to predict localized yielding from the structure SPGs

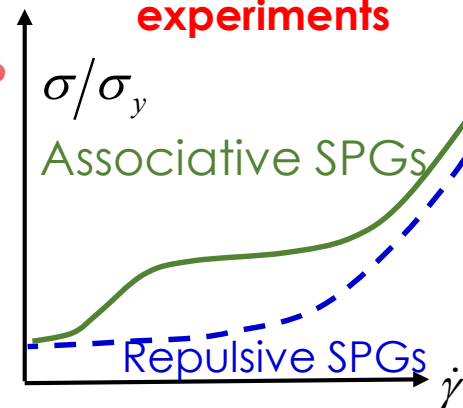
Build models



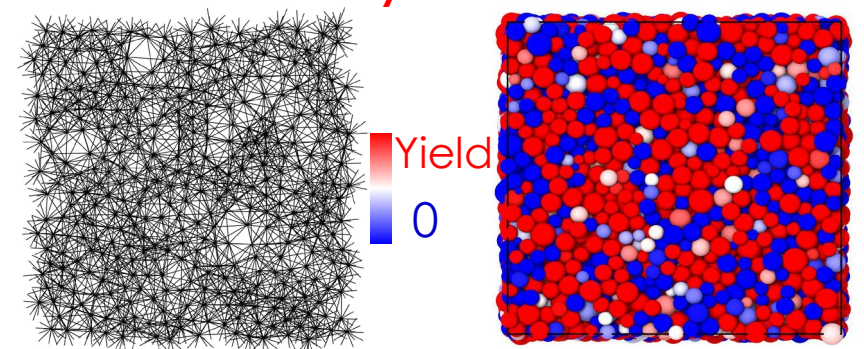
Perform shear simulations



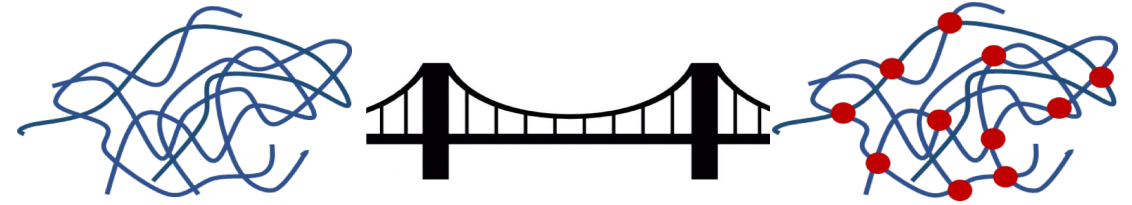
Compare with experiments



Understand the physics and predict dynamics

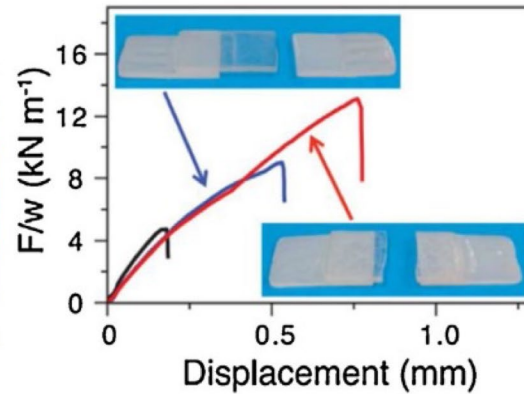
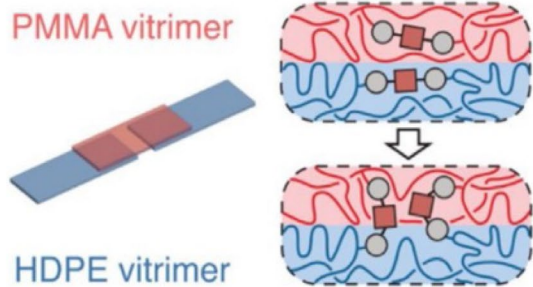


III. Vitrimers: Practical route for reprocessing thermosets



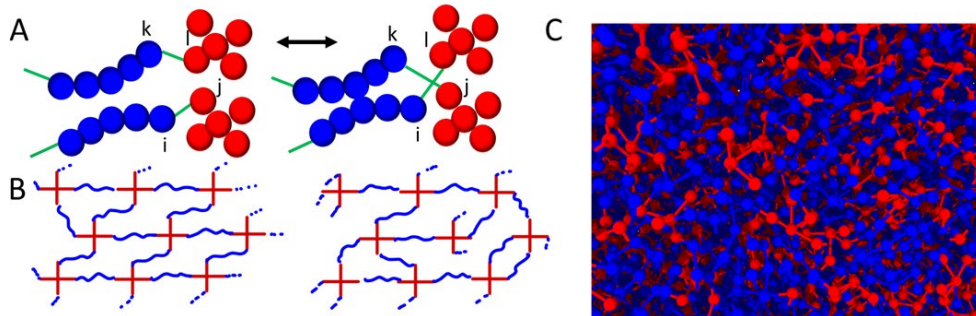
Thermoplastic

Thermoset



Rottger et al., Science, 2017.

Hybrid MD-MC methodology



Rheology

Mechanics

Structure and dynamics

Dynamic moduli

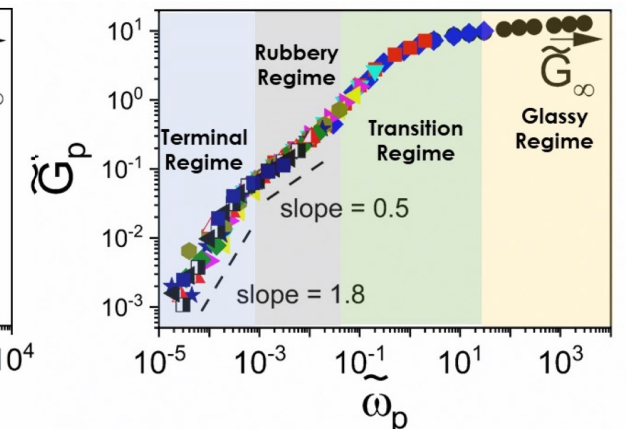
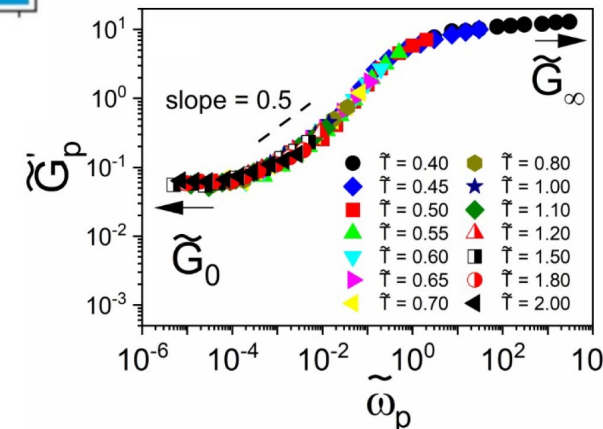
Flow behavior

Stress-strain behavior in linear and nonlinear regimes

Failure and stress distribution

Microstructure under deformation

Deformation-induced dynamics



Perego and Khabaz, Macromolecules., 2021.

Perego and Khabaz, J. Pol. Sc., 2021.

Perego and Khabaz, Macromol. Rapid Commun., 2022.

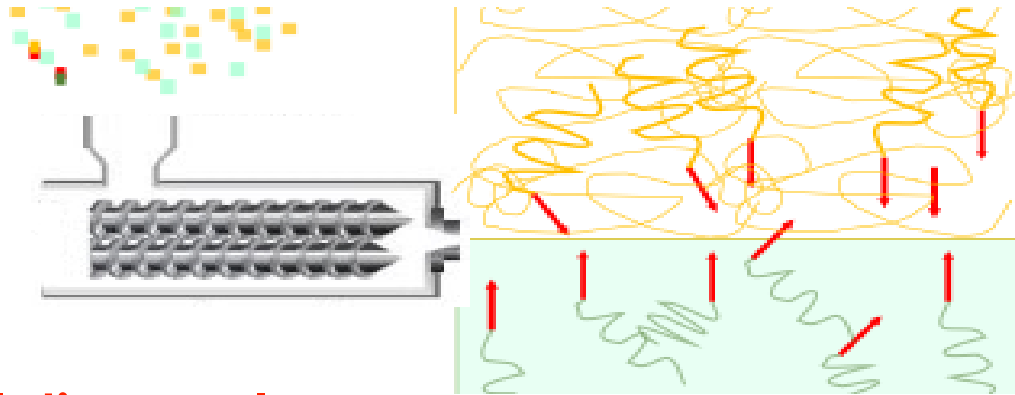
Perego, Lazarenko, Cloitre, and Khabaz, Macromolecules., 2022.

IV. Plastic/rubber recycling: Engineering the interface of incompatible polymer blends



Incompatible polymers in
recycled plastic waste stream

Compatibilizers diffuse and
reinforce the interface



Simulation goals:

- Computational design of interface compatibilizers
- Dynamics of compatibilizers in immiscible blends
- Mechanics of interface

Other components of the project:

- Synthesis
- Physics of crystallization
- Morphology, crystallinity in the boundary of melt-extruded blends and compression molded laminates
- Mechanics
- Processing

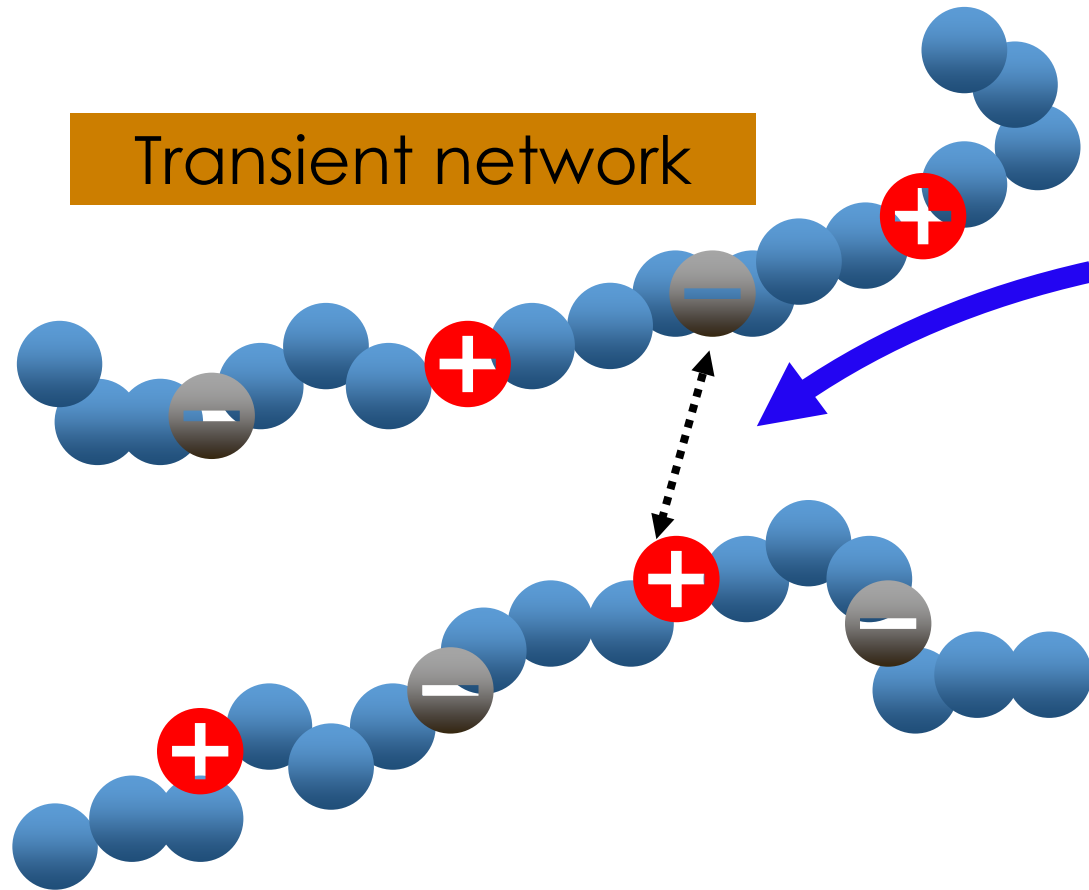
UA: Profs. Jia, Dhinojwala, Khabaz, Jana, Eagan, Miyoshi, and Foster

Industrial collaborator: Braskem



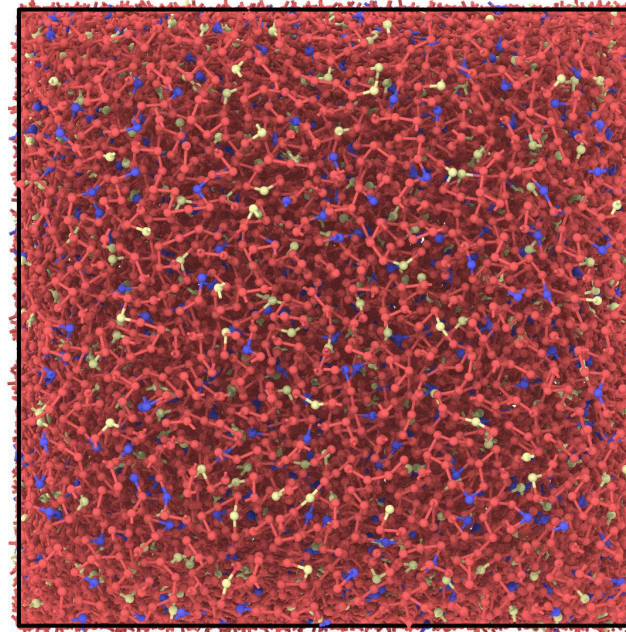
V. Thermodynamics and rheology of shape-memory ionomers

Goal: Understand the mechanism of structural relaxation and rheology



How strong are these bonds?

What is the relaxation time of the bonds?



Collaborators: Prof. Cavicchi