

DoDyNet Kickoff meeting

Soft Matter and Chemistry Lab

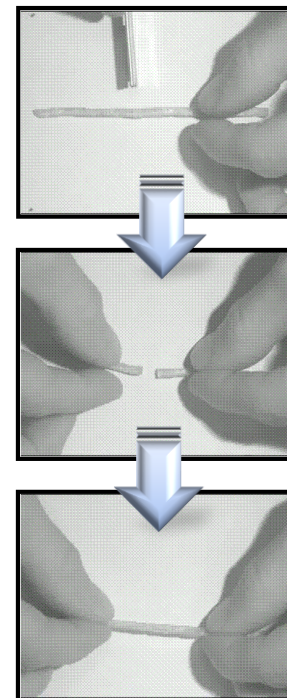
Dynamic Covalent Chemistry and Macromolecular Engineering

Renaud Nicolaÿ



Soft Matter and Chemistry Lab

- Supramolecular Polymers
 - Vitrimers
 - Soft Matter Rheology
- Composites/Hybrid Materials



T = 25°C



T = 90°C



Cordier, P.; Tournilhac, F.; Soulié-Ziakovic, C.; Leibler, L., *Nature* **2008**, 451, 977

Montarnal, D.; Capelot, M.; Tournilhac, F.; Leibler, L. *Science* **2011**, 334, 965

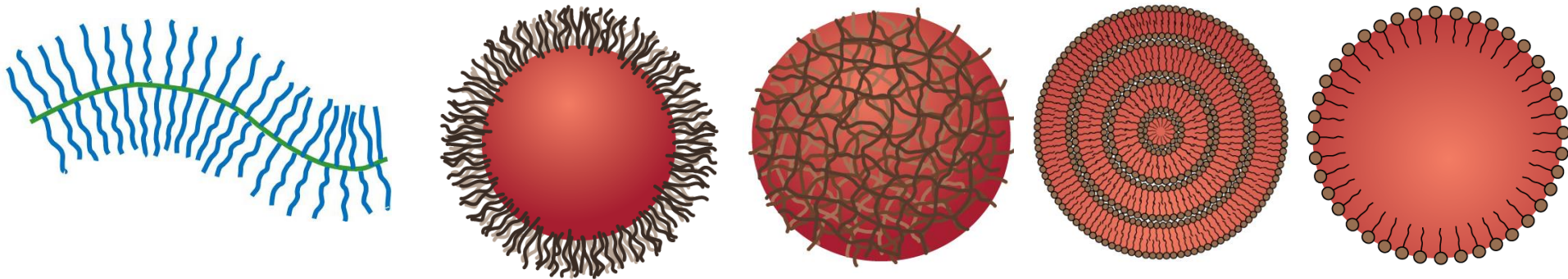
WO2015110642, WO2015110643, WO2016EP50400, FR1661400, FR1661403

Soft Matter and Chemistry Lab

High Solid Dispersions

Polymer-colloids

Soft colloids



Tailoring macroscopic behavior from particle scale properties:

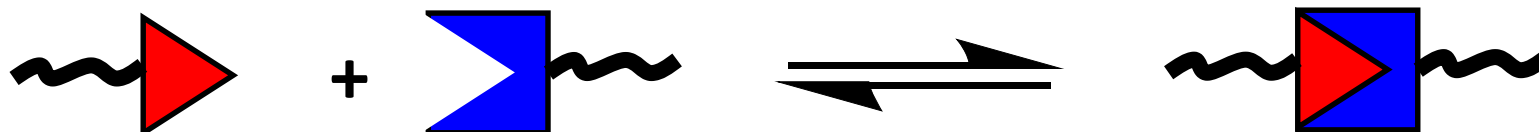
- Yield stress fluids
- Shear-thickening and gelling fluids
- Encapsulation of hydrophobic substances
- Functional polymers for water-soluble formulations



A micromechanical model to predict the flow of soft particle glasses, Jyoti R. Seth, Lavanya Mohan, Clémentine Locatelli-Champagne, Michel Cloitre, Roger T. Bonnecaze, *Nature Materials* 10, 838 (2011)

Reversible and Dynamic Covalent Chemistry

✓ Reversible Covalent Chemistry



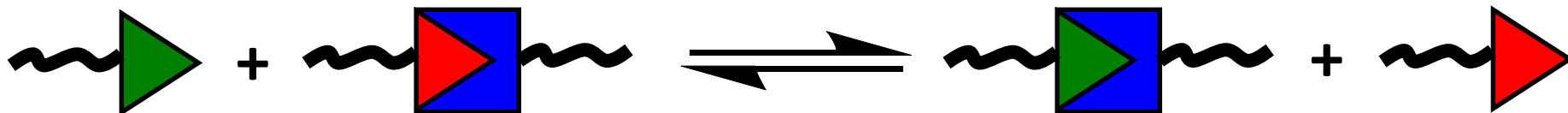
Equilibrium constant

$$K = \frac{k_{\text{formation}}}{k_{\text{rupture}}}$$

Lifetime of the bond

$$\tau \propto \frac{1}{k_{\text{rupture}}}$$

✓ Dynamic Covalent Chemistry



Chemistry and Material Science

**Organic and
Polymer
Synthesis**

Materials

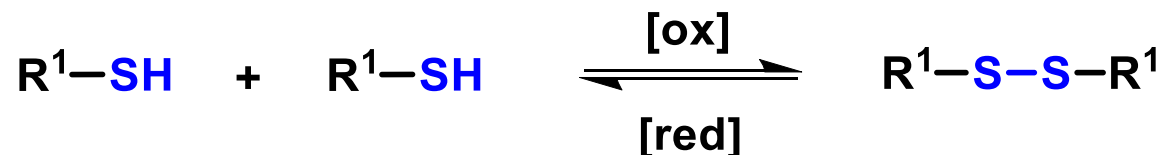
**Reversible and Dynamic
Covalent Chemistry**

**Purification,
Screening,
Detection**

Formulations

Thiol Chemistry

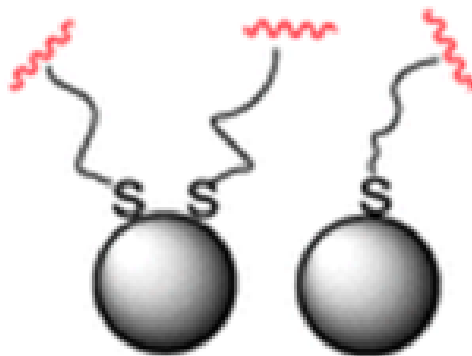
✓ Reversible Covalent Chemistry



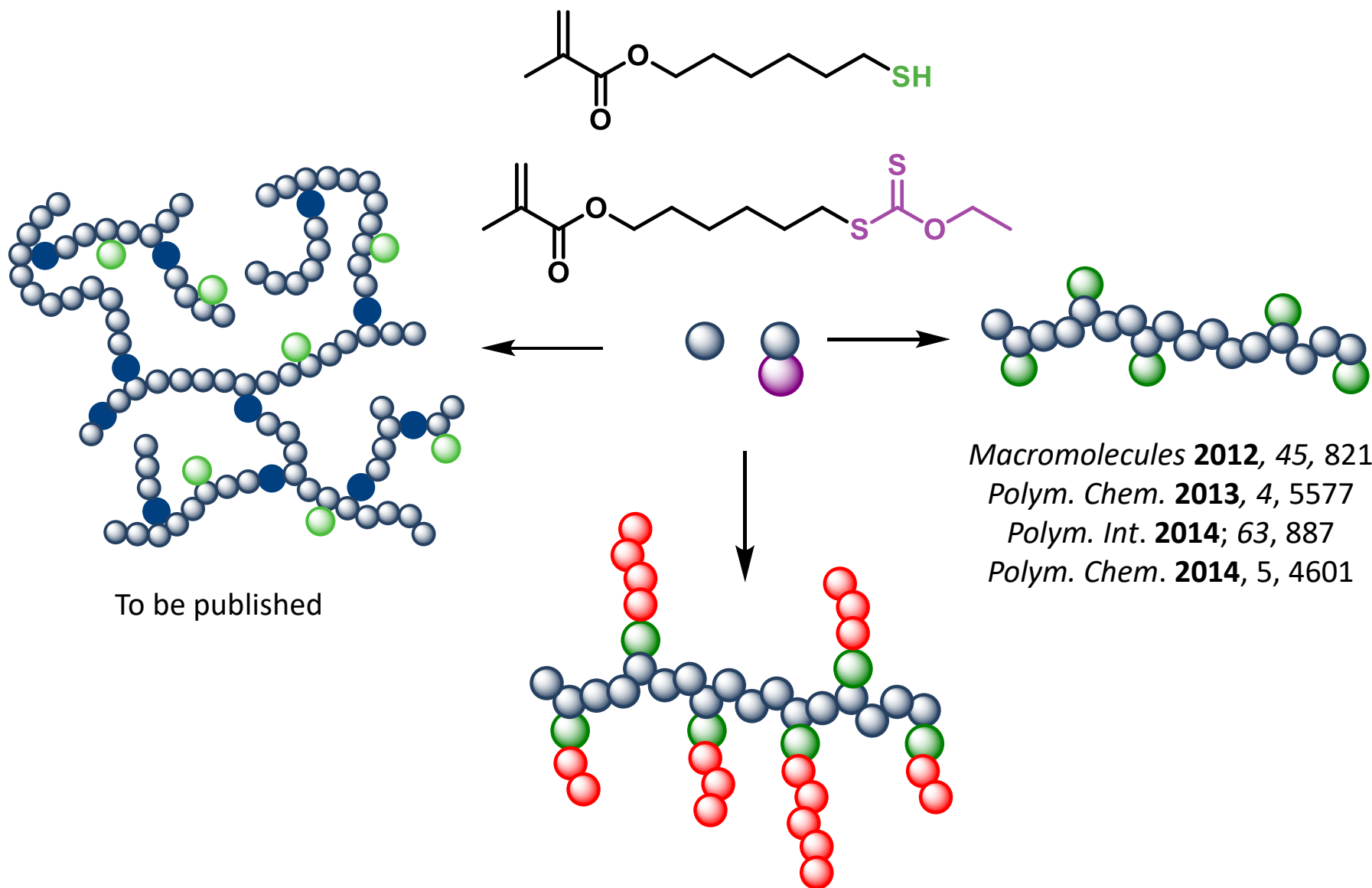
✓ Dynamic Covalent Chemistry



✓ Soft Lewis Base



Polymer Synthesis



To be published

Macromolecules **2012**, 45, 821
Polym. Chem. **2013**, 4, 5577
Polym. Int. **2014**; 63, 887
Polym. Chem. **2014**, 5, 4601

Polym. Chem. **2017**, 8, 5220
Demande de brevet FR1752750

Chemistry and Material Science

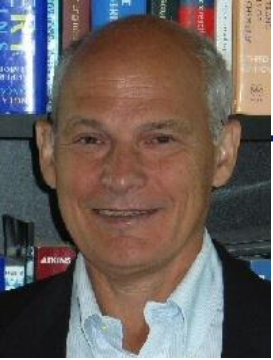
**Organic and
Polymer
Synthesis**

Materials

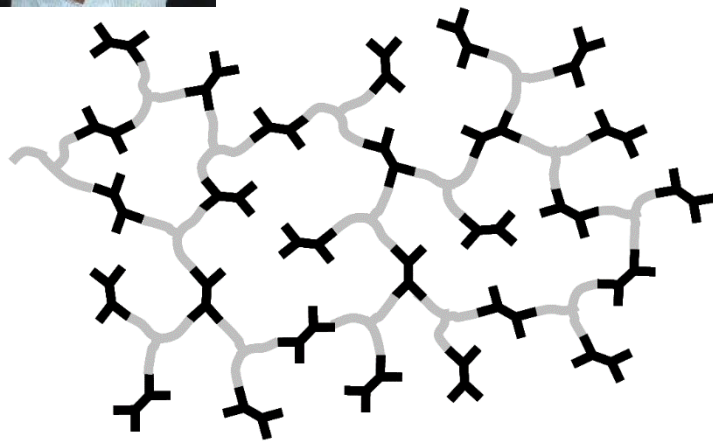
**Reversible and Dynamic
Covalent Chemistry**

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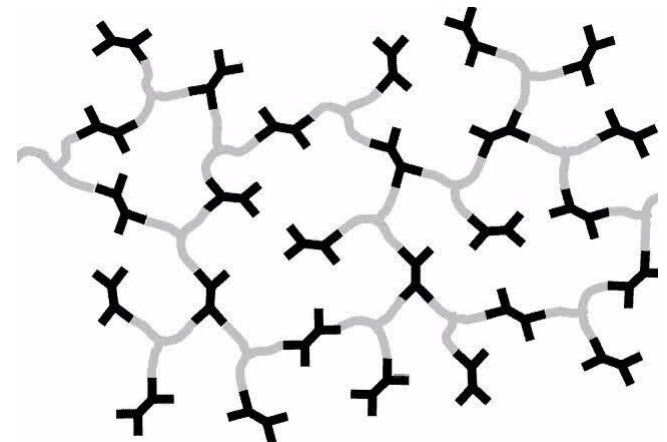
Formulations



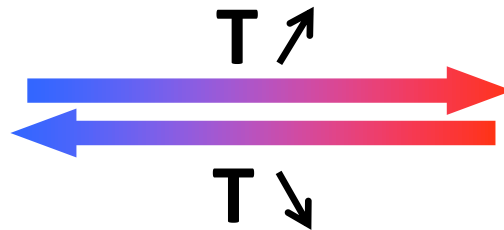
Vitrimers



Frozen Network
Elastic Solid



Dynamic Network
Viscoelastic Liquid



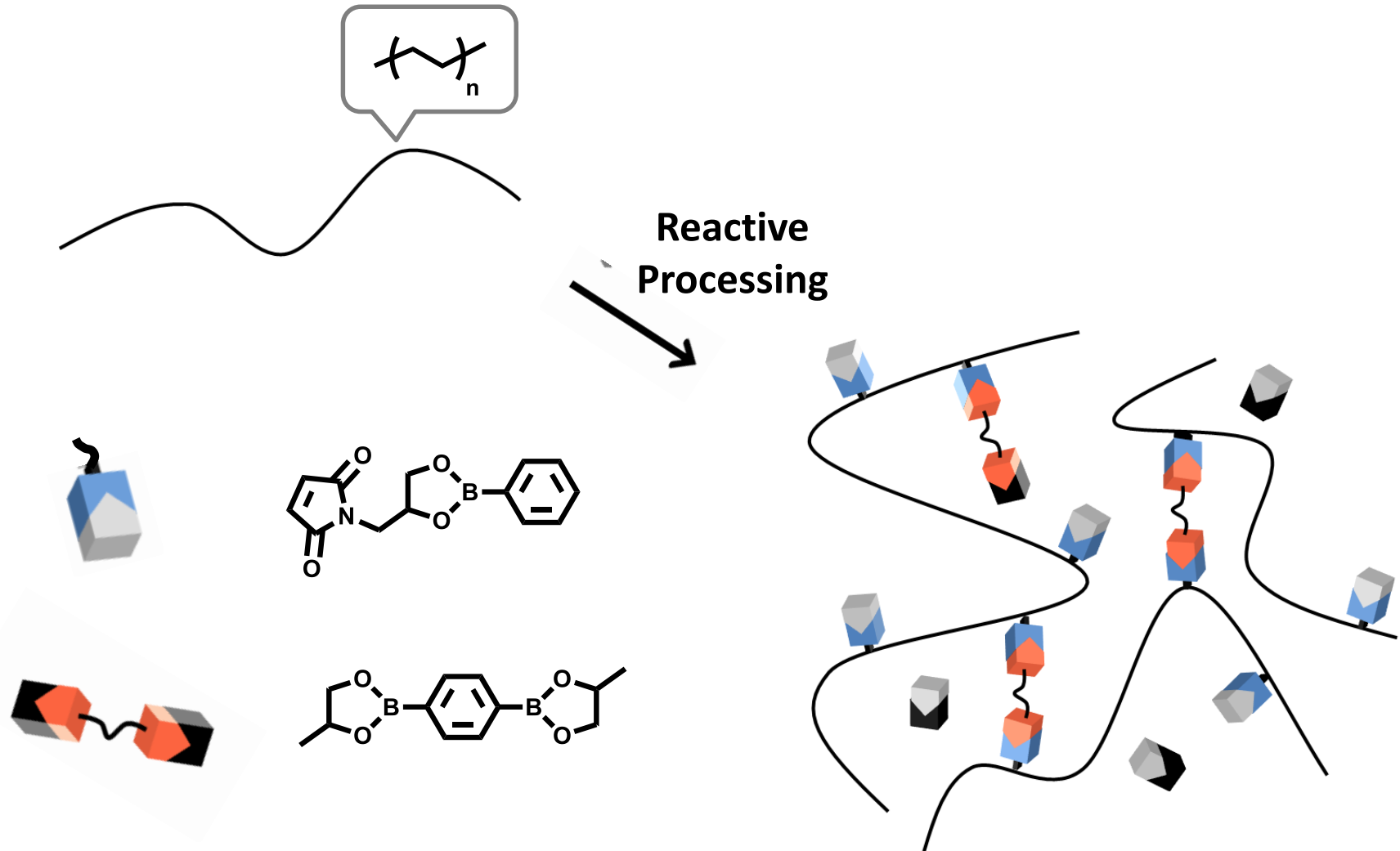
Can flow but remain insoluble

$$\text{Arrhenius: } \eta = \eta_0 \exp(E_a/RT)$$

Montarnal, D.; Capelot, M.; Tournilhac, F.; Leibler, L. *Science* **2011**, 334, 965

Capelot, M.; Unterlass, M. M.; Tournilhac, F.; Leibler, L. *ACS Macro Lett.* , **2012**, 1, 789

Vitrimers from Commercial Thermoplastics



“Simple” additives

HDPE Vitrimers

Processable and Recyclable like Thermoplastics

Injection molding:

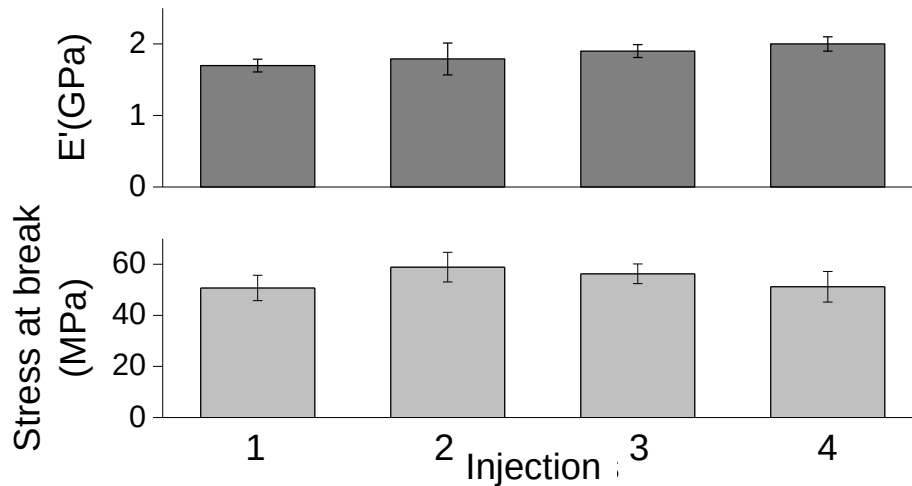
Melt = 200°C, mold = 180°C,
injection at 12 bar for 30 seconds

Compression molding:

150 °C, 10 min



PMMA Vitrimer



PMMA vitrimer injection-molded
and recycled 5 times

Chemistry and Material Science

**Organic and
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**Reversible and Dynamic
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DoDyNet

Networks with two distinct molecular dynamics

- reversible and dynamic chemical crosslinks
- dynamic chemical crosslinks with two different dynamics

Topology, functionality and dynamics of the crosslinks



rheological and mechanical properties of the networks

Structure and homogeneity of the networks (scattering and microscopy techniques)

Use the networks to model the rheological features of double dynamic networks