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SIMULATIONS OF POLYMERS AND POLYMER COMPOSITES

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ABSTRACT

Simulations of polymers and polymer composites are a true challenge due to various physical mechanisms involved, which typically take place at a wide range of time and length scales. The computational techniques should account for the appropriate processes and the relevant range of time and length scales, while, on the other hand, find a reasonable compromise between computational effort and physical accuracy.

The minisymposium **invites contributions in the field of computational treatment of polymers and their composites** based on profound theoretical knowledge and / or experimental evidence. In particular, contributions addressing structure-property relations and coupled multi-physics problems covering, e.g., chemical reactions, biological processes, electromagnetism, or phase transformations, are highly welcome. Furthermore, aspects of uncertainty quantifications related to the aforementioned fields are of specific interest.

Possible contributions may discuss **materials** like thermosets, thermoplastics, elastomers, gels, liquid crystal elastomers, and bio-inspired materials as well as composites and nanocomposites thereof, **structures** in 3d (bulk polymers), 2d (membranes), and 1d (fibres including muscle fibres), **physical states** (melts, solids, semi-crystalline and amorphous polymers) and their evolution (polymerization, curing, and crystallization during processing), **mechanical properties** (viscoelasticity, plasticity, damage, creep, fracture, adhesion, instability), **coupled problems** (piezo-elasticity, electro-elasticity, magneto-elasticity, flexo-elasticity, photo-elasticity, magneto-rheology, crystallization, effects of physical aging and chemical degradation on the mechanical behaviour), and **interfacial phenomena** like surface and confinement effects, interfaces, and interphases.

Simulation techniques fitting into this minisymposium comprise **individual methods** like ab initio approaches, molecular mechanics, molecular dynamics, and finite elements, **coupling**

methods including sequential, hierarchical, and domain-decomposition approaches for atomistic-continuum coupling, coarse-graining, and homogenization, as well as **phase-field methods**, **big-data** and **data-driven strategies**, and **optimization techniques** focusing, e.g., on topology optimization.

Contributions may address **engineering applications**, such as additive manufacturing and 3d printing techniques, composites and nanocomposites for aviation, aerospace, and automotive industry, smart materials and (in-situ) sensors for, e.g., damage detection and moisture measurement, materials, techniques, and design for energy storage purposes like batteries or high-pressure (hydrogen) tanks, life-cycles issues like processing conditions and production methods, service conditions, long-term performance, aging, recycling, and sustainability as well as bio-inspired materials and soft matter design for medical, nutrition, and cosmetics applications.