mODELING AND SIMULATION OF STIMULI-RESPONSIVE ACTIVE MATERIALS

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ABSTRACT

The development of stimuli-responsive or active materials is nowadays a topic of great interest to advanced applications, and is attracting attention from communities spanning engineers, material scientists, physicists and chemists. This intriguing class of materials can undergo microscale structural changes (occurring at the molecular level) in response to environmental conditions, such as pH, temperature, solvent, salt ionic strength, enzymes, light, magnetic and electrical field. These structural modifications may then be translated into sensible macroscale changes that are exploitable for smart actuation and responsiveness.

To properly understand and quantify the functionalities of these new materials, simulation techniques must account for interactions between multiple physics [1]. This could include, for instance, coupling between large deformations, strain rate effect, light diffusion, diffusion of fluids and chemical species, growth, phase changes, etc. Various simulation methods have been proposed to solve this class of problems, namely theoretical methods (TM), multi-physics (chemistry) continuum-based models (CM), molecular dynamics (MD), coarse-grained molecular dynamics (CGMD), dissipative particle dynamics (DPD), Monte Carlo (MC), etc. [2], [3]. The multiscale modelling and simulations of stimuli-responsive materials, especially polymers, could elucidate the molecular-scale mechanisms and provide a guidance for designing new smart materials and improving the existing ones. This mini-symposium welcomes submissions with interest in computational approaches for modeling and simulating active materials (active polymers, dynamic network polymers, liquid crystal elastomers, gels, slide-ring gels, 4D additively manufactured materials, metamaterials, …). The aim of this MS is to gather scientists coming from different fields, interested in modeling active materials across time and length-scale. High-quality and rigorous contributions are particularly welcome.

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