Advancing Materials Development through Multiscale Modelling and Data-Driven approaches in the Safe and Sustainable by Design Framework

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In recent years, the design and development of materials with enhanced properties and reduced environmental impact have become paramount in various industries. Achieving these objectives requires a holistic approach that integrates advanced computational modelling techniques with Safe and Sustainable by Design (SSbD) principles. SSbD emphasizes the proactive identification and mitigation of potential risks associated with materials and products throughout their lifecycle, promoting safety, sustainability, and environmental stewardship.

In this context, multiscale modelling, with its combination of atomistic, mesoscale, and continuum methodologies, plays a pivotal role in elucidating materials safety and sustainability. High-Performance Computing (HPC) infrastructures empower researchers to efficiently perform computationally intensive simulations, analysing complex systems with unprecedented accuracy. This allows for rapid exploration of materials design space, accelerating the discovery of novel materials with tailored properties and performance. Automation of computational tools and workflows, including the integration of artificial intelligence (AI) methods, further enhances efficiency, enabling intelligent decision-making and optimization of design strategies.

In this work, we present the application of this approach in the context of the Horizon Europe project BIO-SUSHY. Our objective is to apply atomistic and coarse-grain molecular dynamics simulations to comprehensively understand toxicity mechanisms in advanced materials. Specifically, we have conducted simulations to explore leaching mechanisms in cellulose surfaces coated with the thermoplastic polymers poly(butylene succinate) (PBS) and poly-β-hydroxybutyrate-co-β-hydroxyvalerate (PHBV). We aim to compare these simulation results with experimental data to provide valuable insights into coating materials for realistic processes. Additionally, we highlight the importance of data integration and automation, combining experimental data, computational results, and predictive AI models to create a unified framework for materials analysis. This research aims to provide insights into coating materials for realistic processes, addressing key challenges for enhanced safety and sustainability.

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