This is how Polymer Informatics can help in designing novel safe-and-sustainable polymers

Society needs safe and sustainable polymers. The current polymer portfolio contains polymers that are either unsafe (e.g. PFAS) or unsustainable, for instance through release of microplastics or through associated GHG-emissions during production. Hence, there are drivers to develop novel polymers. The traditional development of polymers took a century through empirical research, but with sustainability goals set for 2050, a faster approach is needed for fossil-free (CO_2- and biobased) polymers. Fortunately, Polymer Informatics (PI) leverages AI and machine learning to predict properties and design new polymers efficiently.

In this presentation, we will discuss the state-of-the-art of AI for material design and PI in particular. We will highlight current challenges (e.g. data scarcity, polymer fingerprinting) and present TNO's strategy on how to tackle these challenges. We will provide insights into our data collection pipelines, the AI-algorithms we are developing and some initial results of the power of the predictive models in a case study on polymers for textiles. Finally, we will present an outlook on future developments at TNO and discuss options for collaborations with research institutes and various actors in the polymer value chain.