## Bridging from fundamentals to large-scale application - material design and process safety considerations by theory and practice

*Prof. Dr. Markus Busch/Technical University of Darmstadt*

*Thursday, October 9, 2025, 2:30 pm*
*Dupuis Hall, Room 217*

Understanding larger scale production processes, optimizing them or even finding new pathways of production has been a vision in science for decades. Many obstacles have been in the way such as sensing parameters at process relevant conditions or limitations in describing complex systems as well as non-idealities of large-scale reactor implementations.

The high-pressure LDPE process is a mature but still highly relevant one as it serves materials without which modern and green technology would not be feasible. It provides two challenges at a time: The complexity in coupling process conditions and micro-structure of the polymeric material determining the application properties together with harsh reaction conditions of up to 3000 bar and 300 °C. The absence of an upper explosion limit under these conditions set another limit in driving the process. All this manifests at production scales 360kt / year and above per single line.

**Bridging from fundamentals to large-scale application - material design and process safety considerations by theory and practice**

*Prof. Dr. Markus Busch/Technical University of Darmstadt*
*Thursday, October 9, 2025, 2:30 pm*
*Dupuis Hall, Room 217*

**(Cont.)**

Hybrid simulation technologies facilitate process simulations to gather intimate knowledge of the polymeric microstructure that is key to modeling the materials application properties. They are efficient enough to do this on reasonable timescales considering reactor nonidealities in addition. Lab-scale reactor technology being close to industrial application principles such as multi-zone autoclave reactors facilitates model validation in significant broader scope than it would be feasible using industrial reactors only.

Life videography of high-pressure deflagrations on lab-scale facilitates unique insight into unwanted process runaways helping to better understand this phenomenon and its avoidance. For safety devices systematic full-scale testing is the gold standard. However, this is out of reach for such types of decomposition reactions. Full-scale testing of inert systems and their good description by models, then being downscaled to lab-scale replicates provides the potential to reverse the process for high-pressure deflagration reactions from lab- to full-scale.