

International Conference and Advanced Workshop on Modelling and Simulation of Complex Systems



Contribution ID: 76

Type: **not specified**

Computational analysis of enzymatic processes in polymer degradation

Monday, 27 May 2024 10:10 (25 minutes)

Biodegradability of materials and material building blocks, such as polymers, monomers, polymer crosslinkers is a long lasting question related to environmental issues. The improvement of polymeric materials for biological degradation is a field of active research with many challenges. A newly developed computational model can sufficiently describe the oxidative degradation of polymer building blocks as they occur at mono oxygenase enzymes. This computational model helps to understand the properties of degradable materials and to identify potentially biodegradable building blocks for polymer chemistry.

Presenter: Dr LEVEN, Matthias (Covestro Deutschland AG)