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Computational model integration across SSbD dimensions on advanced materials and chemicals: development driven by industry and innovators needs

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Abstract

Safe-and-Sustainable-by-Design (SSbD) advanced materials and chemicals (AMCs) are a central requirement for reaching the ambitious goal of making Europe the first digitally enabled circular, climate-neutral, and sustainable economy. Novel AMCs need to provide the high functionality required for their advanced applications, whilst simultaneously exhibiting improved safety and sustainability performance considering the complete value chain and life cycle, as outlined in the SSbD framework proposed by the EU Joint Research Centre [1], adopted in the Commission Recommendation of 8 Dec. 2022 [2], and supplemented by methodological guidance [3]. To facilitate adoption by industry and, by doing so, foster the twin green and digital transition of Europe's economy, the "PINK - Provision of Integrated Computational Approaches for Addressing New Markets Goals for the Introduction of Safe-and-Sustainable-by-Design Chemicals and Materials" Project aims to produce innovative modelling software and integrated workflows for the development of AMCs, which are combined into an industry-ready open innovation platform, the PINK In Silico Hub (PINKISH). PINK takes a holistic "by-Design" approach targeting the primary goal to satisfy the needs of industry, as implementing SSbD presents the multi-objective optimization problem to balance the four requirement categories functionality, cost-efficiency, safety, and sustainability. Starting from two industry-driven developmental Case Studies (CSs) PINK has established three scenarios that operate at different development stages within the industrial AMC innovation pipeline: *Scenario 1* at business opportunity stage where multiple candidates can be generated *in silico* and potentially later arising sustainability constraints are to be determined by predictive modelling in parallel to functional performance testing (correlating with Tier 1 SSbD assessment); *Scenario 2* at innovation development stage defined by one lead structure identified and some information is available (performance and partially safety and sustainability) with *in silico* tool-based modifications going on and sustainability criteria being evaluated (Tier 2); and *Scenario 3* at later material design stages where more data for several dimensions becomes available (Tier 3). Depending on CS requirements and scenarios envisioned, PINK addresses elements for all SSbD dimensions, employing CS-customized *in silico* tools, continuously improving the confidence in the predictions over multiple design cycles by producing new knowledge on a constantly reduced set of better performing candidates for replacing substances of concern. Industry readiness shall be guaranteed by improving usability, practicability, user experience, data provenance, documentation, and

security. Pulling in further CS from different materials sectors the CS-customization of tools is gradually decreased by an innovators-guided generalization approach to enable broadening the applicability of integrated computational workflows to a wider range of advanced material innovation markets.

References

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Personal sketch:

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