



This project received funding from the European Union's Horizon Europe research and innovation programme under grant agreement n° 101177608. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union. Neither the European Union nor the granting authority can be held responsible for them.

# Implementing SSbD in chemicals and materials value chains: Challenges & opportunities

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BNN Annual Forum 2025 – Linz

Disclaimer: no specific details on the content of the cases can be given



#### Background





Become climate-neutral by 2050



Protect human life, animals and plants, by cutting pollution



Help companies become world leaders in clean products and technologies

#### Some EU policies:





• Circular Economy Action Plan

• Biodiversity strategy

• Critical Raw Materials Act

• EU Goals for Air, Soil and Water

• Farm to Fork strategy

• Fit for 55 Package

...call for <u>twin green and digital transition</u> to a sustainable, climate-neutral and circular as well as globally competitive and resilient economy



Help ensure a just and inclusive transition

https://research-andinnovation.ec.europa.eu/funding/fundingopportunities/funding-programmes-and-opencalls/horizon-europe/eu-missions-horizon-europe\_en

### Background on SSbD





PLANETS will demonstrate the applicability of the SSbD framework in 3 real industrial case studies (plasticizers, flame retardants, surfactants), developing safer & more sustainable alternatives to critical chemical materials!



## What is SSbD? → That is the Challenge!

Safe and Sustainable by Design

#### Hazard x exposure = risks

- Human health effects
- Worker/consumer exposure
- Environmental exposure

#### Life cycle impacts

- Environmental (climate, biodiversity, resources, etc.)
- Social (working conditions, human rights, etc.)
- Financial (e.g. TCO, LCC)

#### **Functionality**

- Chemical, material, product, process, etc.
- Trade-offs between dimensions
- End-of-life

SSbD → holistic view, entire product lifecycle

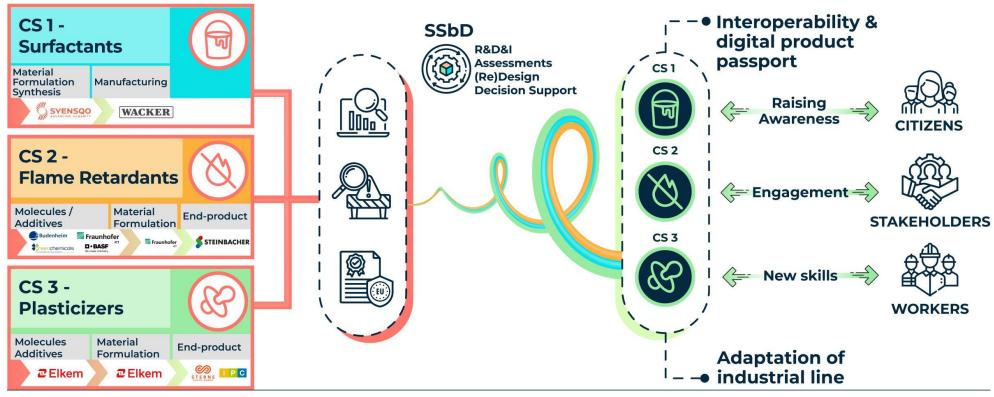


# PLANETS' case studies for implementing SSbD

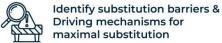








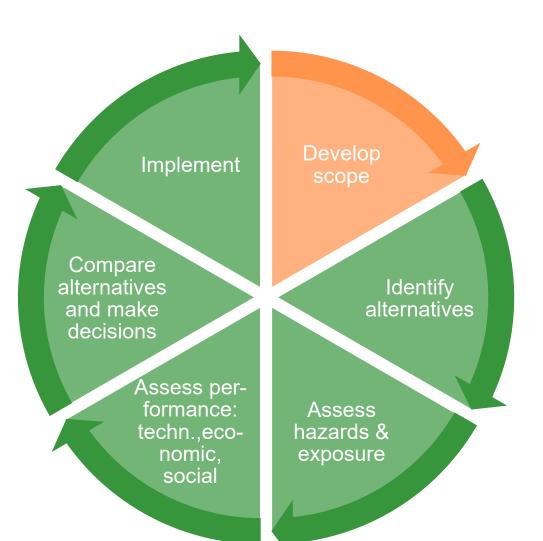






## For SSbD you need a plan → Scoping





The scoping analysis determines the boundaries and provides focus for the SSbD assessment by answering the questions:

- (Re)design definition: WHY (WHAT)
- System definition: WHAT
- Actors in the life cycle: WHO
- The assessment: HOW

Gallegos GML, et al., 2025, <a href="https://doi.org/10.1016/j.csbj.2025.07.030">https://doi.org/10.1016/j.csbj.2025.07.030</a>

#### Decision on acceptable alternatives



#### ... a process of integrating information; a multi-criteria approach

#### **Criterion**

Physiochemical properties

Hazard characteristics

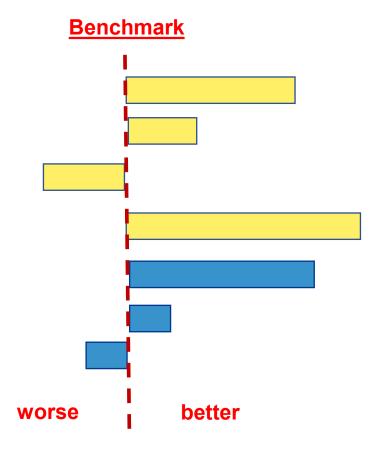
Intrinsic exposure potential

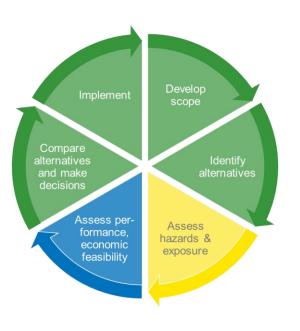
Potential lifecycle trade-offs

Technical feasibility

**Economic feasibility** 

Availability of competences

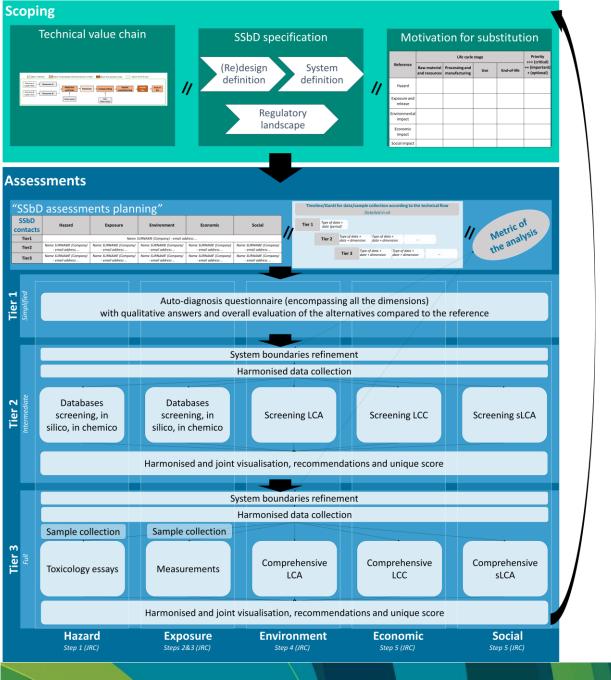




### Assess trade-offs & consider data gaps/quality



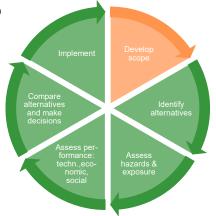
Alternative	Evaluation criteria	Weights	Data gaps / quality	Score	Total	Ranking
A1	X X X X X X X		X	1 2 2 0 3 -1	1	2
A2	x x x x x x		x	3 1 2 -2 3 2	3	1
A3	X X X X X		x	2 -2 2 0 0 3	0	3



WHY? WHO? WHAT?







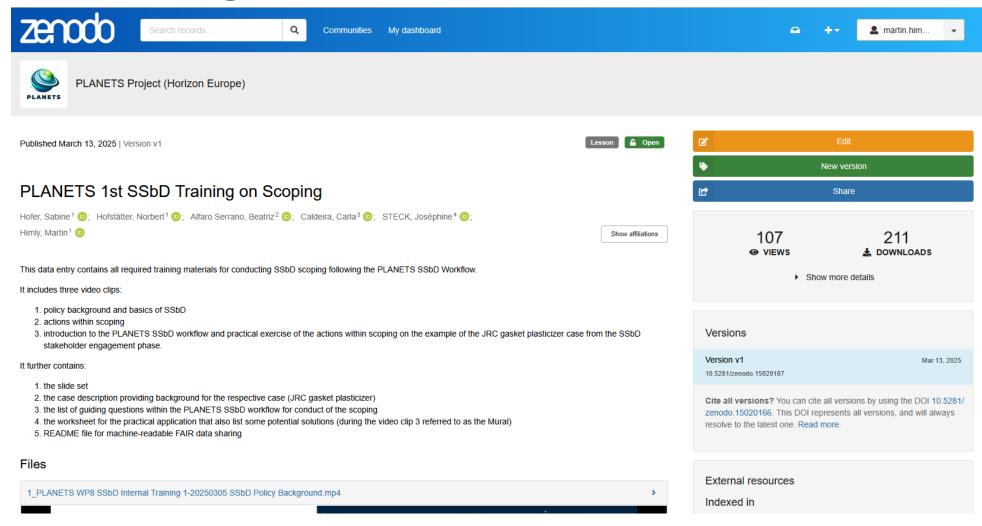
# The PLANETS generic SSbD workflow

A two phases approach aiming to guide the CS through SSbD:

- Scoping Formalise the system under study to ensure efficient SSbD assessments
- Assessments Conduct evaluations of the alternatives in comparison to a benchmark

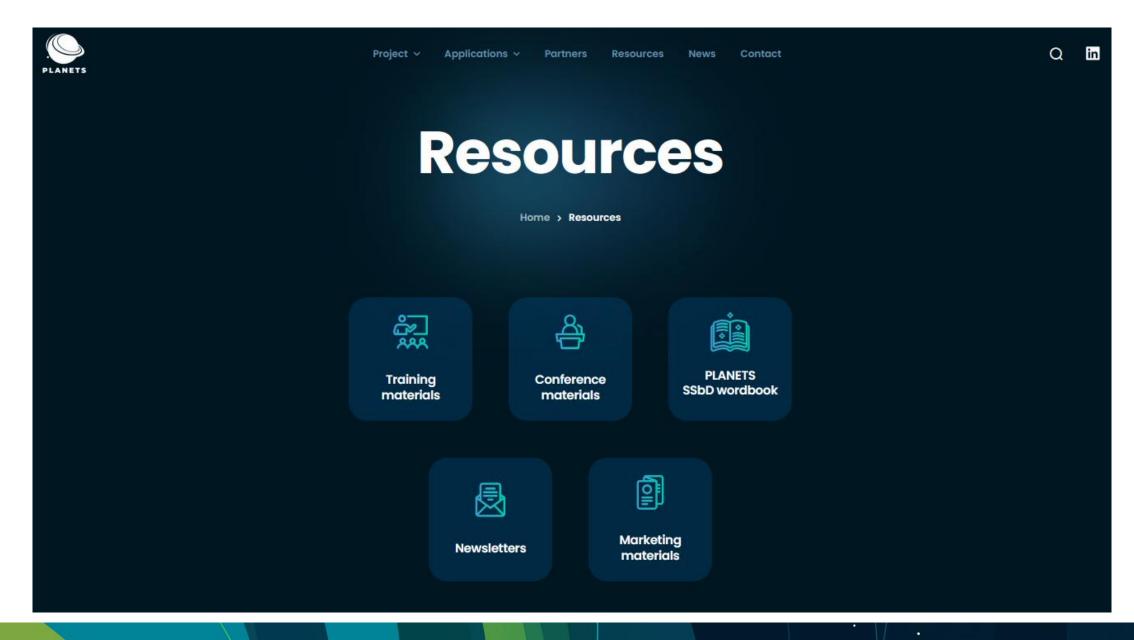
## PLANETS' Scoping workflow at Zenodo





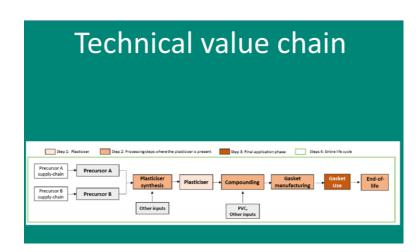
Hofer, S., Hofstätter, N., Alfaro Serrano, B., Caldeira, C., Steck, J., & Himly, M. PLANETS 1st SSbD Training on Scoping. <a href="https://doi.org/10.5281/zenodo.15020167">https://doi.org/10.5281/zenodo.15020167</a>







Objective 1: Define the technical value chain



The technical value chain refers to the series of interconnected processes and stakeholders that contribute to the creation, development, and delivery of the final product.

plastisol liner

It defines the roles of technical actors and outlines their contributions at each stage of the product life-cycle, from initial concept through design, production, and maintenance. Each link in the chain adds technical value by refining processes, improving efficiency, and ensuring the quality and functionality of the end product.

Link to material: <a href="https://doi.org/10.5281/zenodo.15020167">https://doi.org/10.5281/zenodo.15020167</a>

# Objective 2: Motivation for re-design





Mc	Notivation for substitution					
		Priority				
Reference		Processing and manufacturing	Use	End-of-life	+++ (critical) ++ (important + (optional)	
Hazard						
Exposure and release						
Environmental impact						
Economic impact						
Social impact						

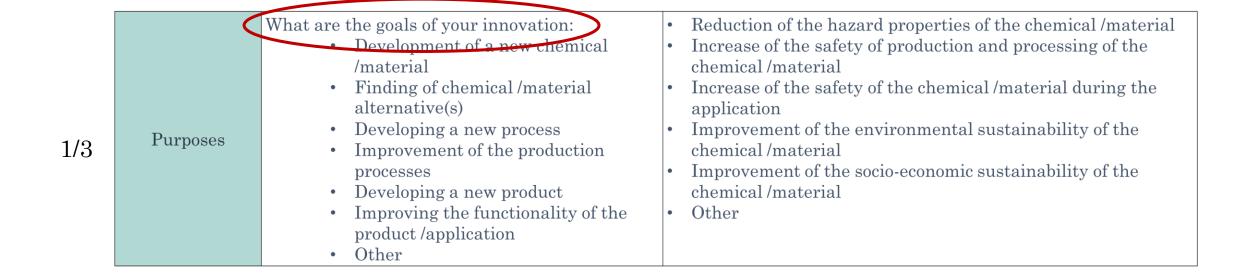
		Priority +++ (critical)			
Reference	Raw material and resources	Processing and manufacturing	Use	End-of-life	++ (important) + (optional)
Hazard					
Exposure and					
release					
Environmental					
impact					
Economic impact					
Social impact					

Link to material: <a href="https://doi.org/10.5281/zenodo.15020167">https://doi.org/10.5281/zenodo.15020167</a>



# Objective 3: (Re)Design and system boundaries definition

(Re)design definition System definition



Link to material: <a href="https://doi.org/10.5281/zenodo.15020167">https://doi.org/10.5281/zenodo.15020167</a>



# Objective 3: (Re)Design and system boundaries definition

(Re)design definition System definition

What are the SSbD principles relevant for your CS that should be assessed:

• Material efficiency

• Minimise the use of hazardous chemicals or materials

• Design for energy efficiency

• Use renewable sources

• Prevent and avoid hazardous emissions

• Design for end of life

• Consider the whole life cycle

• Other principles (please specify)

Link to material: <a href="https://doi.org/10.5281/zenodo.15020167">https://doi.org/10.5281/zenodo.15020167</a>



# Objective 3: (Re)Design and system boundaries definition

(Re)design definition

System definition

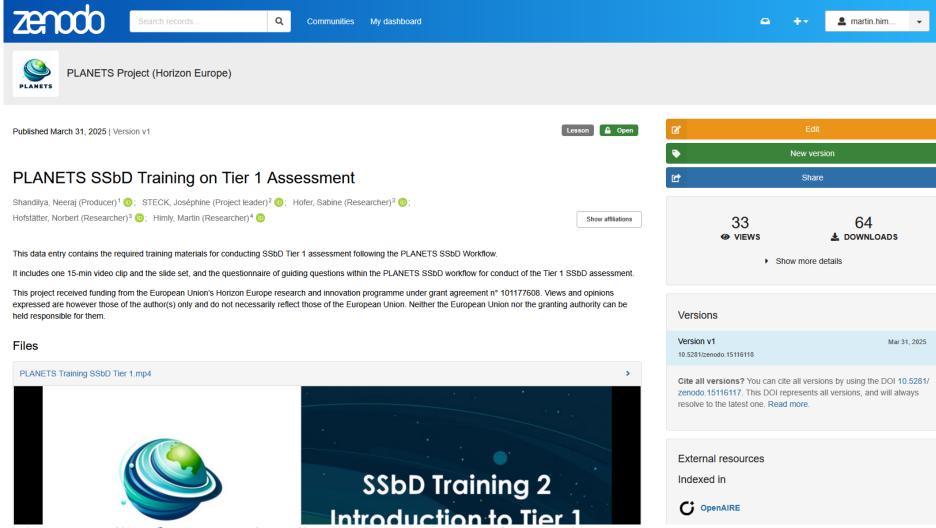
Molecular (re)design	Process (re)design	Product (re)design
Is there any existing chemical/material that can be used as a reference to compare the results of the SSbD study?  If no reference chemical/material has been selected, the reference might be chosen with one of the following aspects:  • Chemical/material with similar structure  • Chemical/material fulfilling the same function  • Representative Chemical/material as for the definition of Representative Product in the PEF method  • Other criteria to define the benchmark At which Technology Readiness Level (TRL) is chemical/material under development?	Does the improvement of the process require a new technology? If yes, at which Technology Readiness Level (TRL) is the new technology(ies) for the process improvement? Provide information about the new technology needed for the improvement of the process, for instance the characteristics, the energy and auxiliaries consumed, its emissions and waste generated	Does the (re)design of the product/application involve a new application? If yes, at which Technology Readiness Level (TRL) is the new technology(ies) for the process improvement? Provide information about the new technology needed for the improvement of the product/application

Link to material: <a href="https://doi.org/10.5281/zenodo.15020167">https://doi.org/10.5281/zenodo.15020167</a>

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#### **PLANETS' Tier 1 at Zenodo**





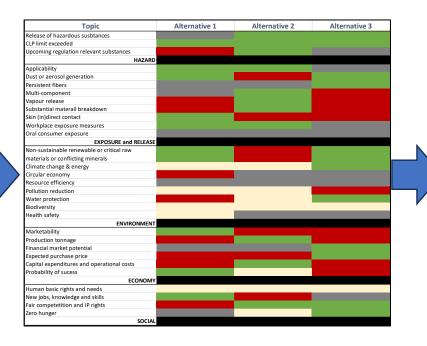
Shandilya, N., Steck, J., Hofer, S., Hofstätter, N., & Himly, M.

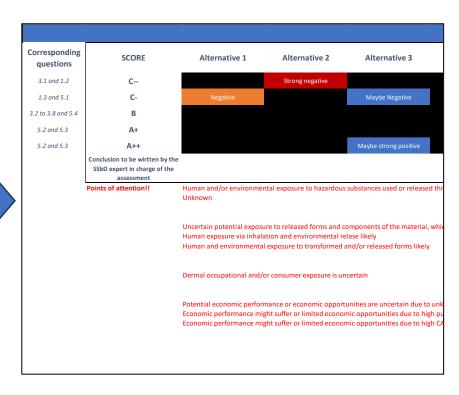
PLANETS SSbD Training on Tier 1 Assessment. <a href="https://doi.org/10.5281/zenodo.15116118">https://doi.org/10.5281/zenodo.15116118</a>

	Dimension 1: Hazard	Reference	Alternative 1	Alternative 2	Alternative 3
	Is the human and/or environmental release of hazardous substances (Substances of very high concern, Equivalent level of concern, Substances of				
1.1	concern, or hazard band C, D, or E) likely at any stage of the product's life	Yes	Unknown	No	No
	cycle?				
	Is it likely that the CLP limit for hazardous substances will be exceeded in the final application, with a concentration greater than 0.1% w/w?	Unknown	No	No	No
	final application, with a concentration greater than 0.1% w/w?				
	Are substances which are relevant for upcoming regulations and/or industry/customer specific requirements likely to be present? e.g. SoCs present				
	in ESPR relevant products substances on Restriction Road Man			No	
1.3	(https://ec.europa.eu/docsroom/documents/49734) or on the chemicals	No	Yes	No	Unknown
	convention list.				
2.1	2: Release and exposure	No	Yes	Yes	Unknown
	Do you identify the potential use/applicability of the final material/product?  At any life cycle stage, is your material or product in powder form and/or is it				
	possible that dust or aerosols are released?	No	No	Yes	No
2.2a	If yes, does your material contain rigid, persistent fibres (length > 5 $\mu m$ and	Unknown	Unknown	Unknown	No
2.3	diameter < 3 μm)?	Yes	Unknown	No	Yes
	At any life cycle stage, is your material or product in a liquid/yanour (with				
2.4	vapour pressure > 1 Pa) and/or is it possible that vapours are released?	No	Yes	No	Yes
2.5	Is there a possibility of substantial material breakdown during production, use	No	Yes	No	Yes
	and/or end of life?  Is there a possibility of (in)direct contact with worker and/or consumer skin?	No	No	Yes	Yes
		No	Yes	Yes	Unknown
		Unknown	Unknown	Unknown	Unknown
	3: Environmental impact				
	Are non-sustainable renewable raw materials or conflicting minerals or critical		No	Yes	No
	raw materials used during production? What is the impact of the new material or product compared to the		140		
	conventional material or product on the following sustainable development				
3.2	category: Climate change mitigation & energy conservation?* (Click on this cell		Equal	Equal	Positive
	for more information)				
	What is the impact of the new material or product compared to the				
3.3	conventional material or product on the following sustainable development category: Circular economy?* (Click on this cell for more information)		Negative	Unknown	Unknown
	category: Circular economy?* (Click on this cell for more information)				
	What is the impact of the new material or product compared to the				
	conventional material or producton on the following sustainable development		Unknown	Unknown	Unknown
	category: Resource efficiency?* (Click on this cell for more information)				
	What is the impact of the new material or product compared to the				
	conventional material or producton on the following sustainable development		Equal	Equal	Negative
	category: Pollution reduction?* (Click on this cell for more information)				
	What is the impact of the new material or product compared to the				
3.6	conventional material or producton on the following sustainable development		Negative	Equal	Positive
	category: Water protection?* (Click on this cell for more information)				
	What is the impact of the new material or product compared to the				
3.7	conventional material or product on the following sustainable development		Equal	Equal	Equal
	category: Biodiversity protection?* (Click on this cell for more information)				·
	What is the impact of the new material or product compared to the				
	conventional material or product on the following sustainable development		Equal	Unknown	Unknown
	category: Health safety?* (Click on this cell for more information)				
	4: Economic performance				
	Is the marketability of the new material or product better or equal to the				
	benchmark due to, for instance, improved or new functionality or a clear image		Yes	No	No
	advantage? (Click on this cell for more information)  Is the foreseen production tonnage of the new material or product ≥ 1 tonne				
	per year? Calendar year is from 1 Jan to 31 Dec.		No	Yes	No
4.3	Is the foreseen market potential of the new material or product ≥ 1M€ in		Unknown	Unknown	Yes
	Europe?  Is the (expected) purchase price per unit of the new material or product lower				
	or equal to the benchmark?		No	No	Yes
	Are the capital expenditures and operational costs (e.g. maintenance, energy				
4.5	use) during the production and/or use phase of the new product or application		No	Yes	No
	lower or equal to the benchmark?  What is the aggregated probability of success to manufacture of the new				
	product on a commercial scale?		>50%	10% to 50%	<10%
	5: Social				
	Compared to the benchmark, does the new material or product development				
	lead to the deterioration of basic rights & needs of the workers, consumers, including children, and on the local community? (Click on this cell for more		No	No	No
	information)				
	Compared to the benchmark, does the new material or product development				
	lead to an improvement in creating new jobs, development of new skills,		Yes	No	Unknown
	knowledge and employability, society's economic/technologic/sustainable development?				
	Compared to the benchmark, does the new material or product development				
5.3	allow for fair competition, good supplier relationships and respect of		No	Yes	Yes
	intellectual property rights?				
5.4	What is the impact on the following sustainable development category: zero hunger?* (Click on this cell for more information)		Unknown	Equal	Positive
	S				

#### Tier 1 assessment tool







### Gaps identified & actions prioritized



- 1. Confidentiality issues of open access tools for hazard assessment (Vega & OECD QSAR Toolbox can be downloaded, instructions how to use); Diamonds tools, Stoffenmanager, etc.
- 2. Functionality inclusion to SSbD assessment procedure
- 3. Methodology:
  - Clustering procedure to be defined (in case of many alternatives)
  - Integration of risk assessment with LCA: comparative vs absolute dilemma
  - Harmonized data collection (metrics, etc.)
  - Uncertainty management
  - Multi-criteria decision analysis (MCDA): transparent decision points, weighting, optimization under uncertainty, stakeholders, etc.

### Gaps identified & actions prioritized



- 4. Simplified (Tier 1) assessment refinement:
  - Decision tree needs to be made adaptable (CRM, CLP limits, etc.)
  - The simplified assessment is not suitable for **differentiation in narrow design space** (applicability domain); it should be done in project teams of a single stakeholder (e.g., innovators and others, incl. business)
  - Care with showstoppers, because it may kick out the whole preselected design space (how to compensate trade-offs?)
  - Need for weighting of aspects carried in from scoping
  - Need for an intra-tier 1 iterative assessment approach rather than a straightforward strategy to follow more closely the intrinsic learning curve of any innovation

#### • 5. Tools:

- Issues of by-products to be included in the SSbD assessment (storage, manufacture, etc.)
- Tool for hazard prediction of new substances missing (e.g., read-across incl. uncertainty captured; OECD QSAR Toolbox)

### Gaps identified & actions prioritized



#### 6. Scoping:

- Use phase definition to be described
- Stakeholder perspective depending on the position in the value chain
- Concept of exposure scenarios not clear enough
- Better goal description/instructions of "Motivation for re-design"
- Needs a multi-disciplinary approach
- Must capture existing policy hard facts and minimum requirements
- Relies on (and should lead to) a common understanding of the system under investigation
- Link between scoping phase and assessment phase → essential outcomes from scoping
  phase have to directly flow into the assessment phase
- **Shared mindset** necessary that scoping has a descriptive function of the existing system (value flow, boundaries, policies, priorities, decision rules, weighting), while tiered assessment is investigative going beyond that and with inclusion of the alternatives.



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Ze Zenodo

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