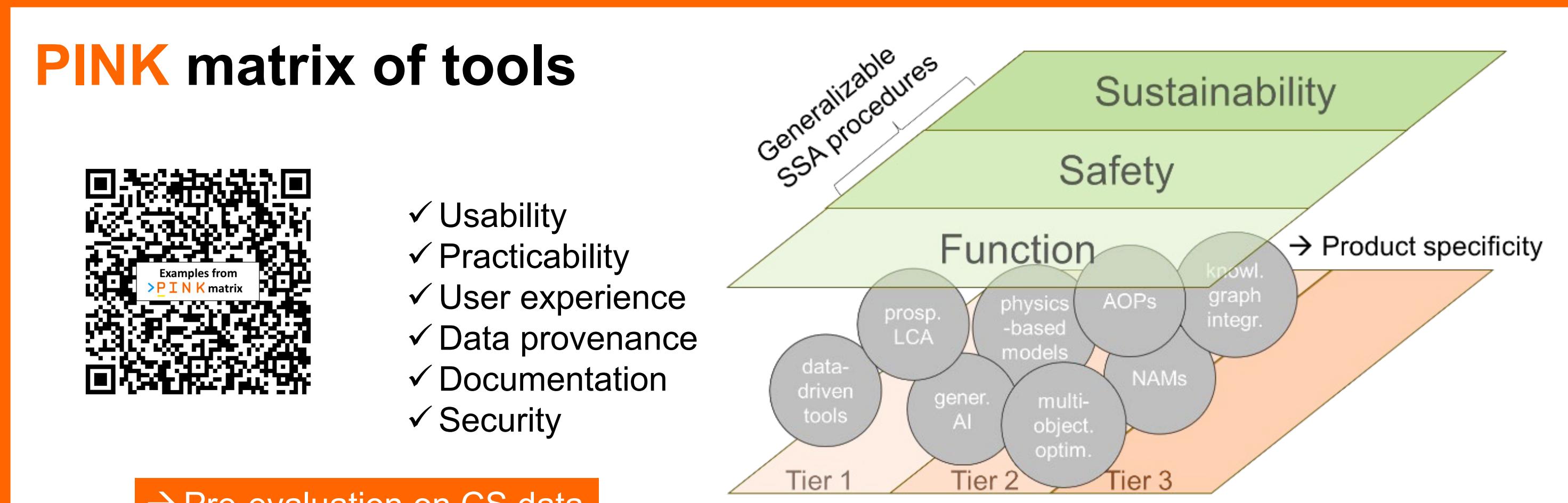
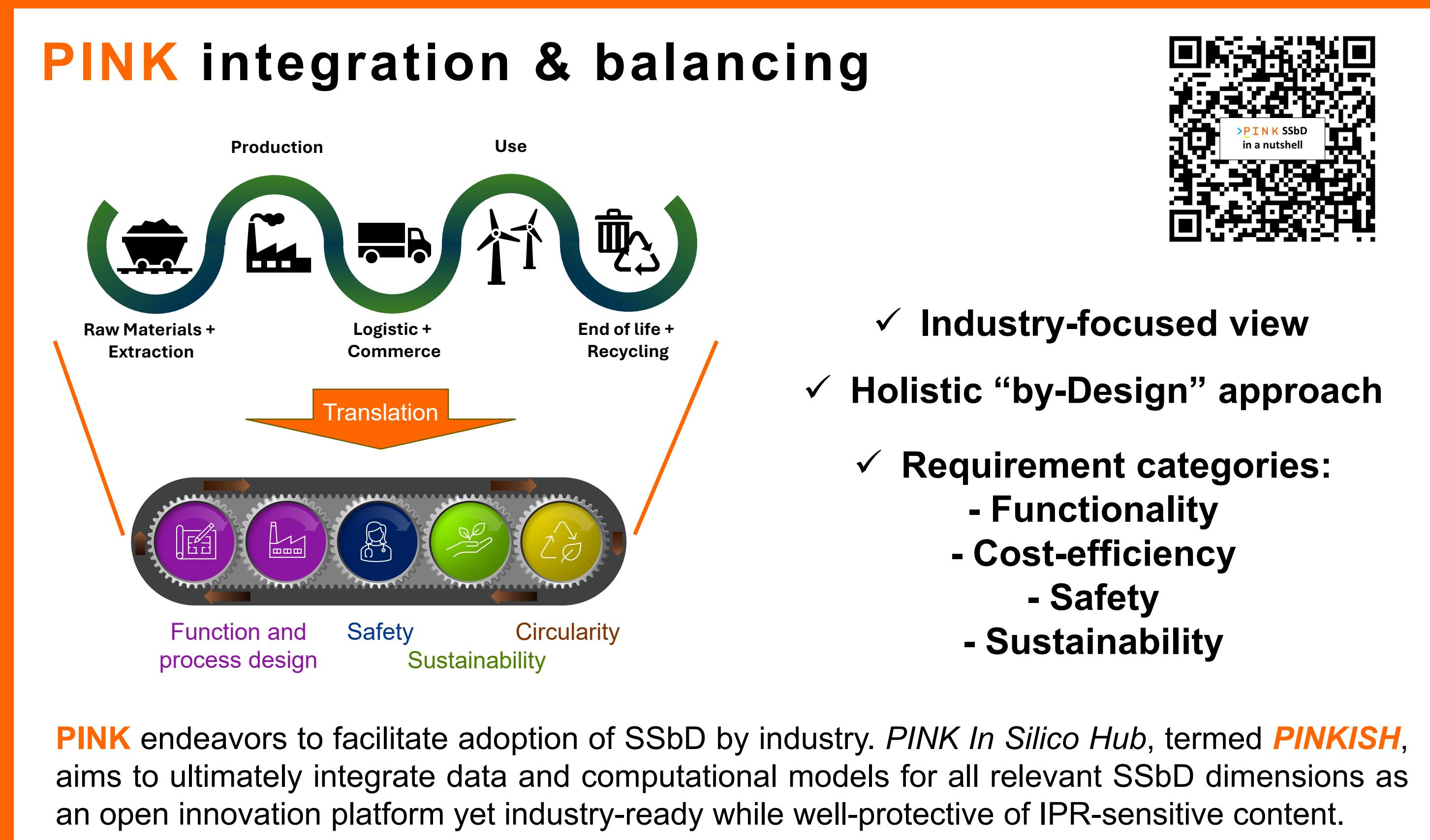


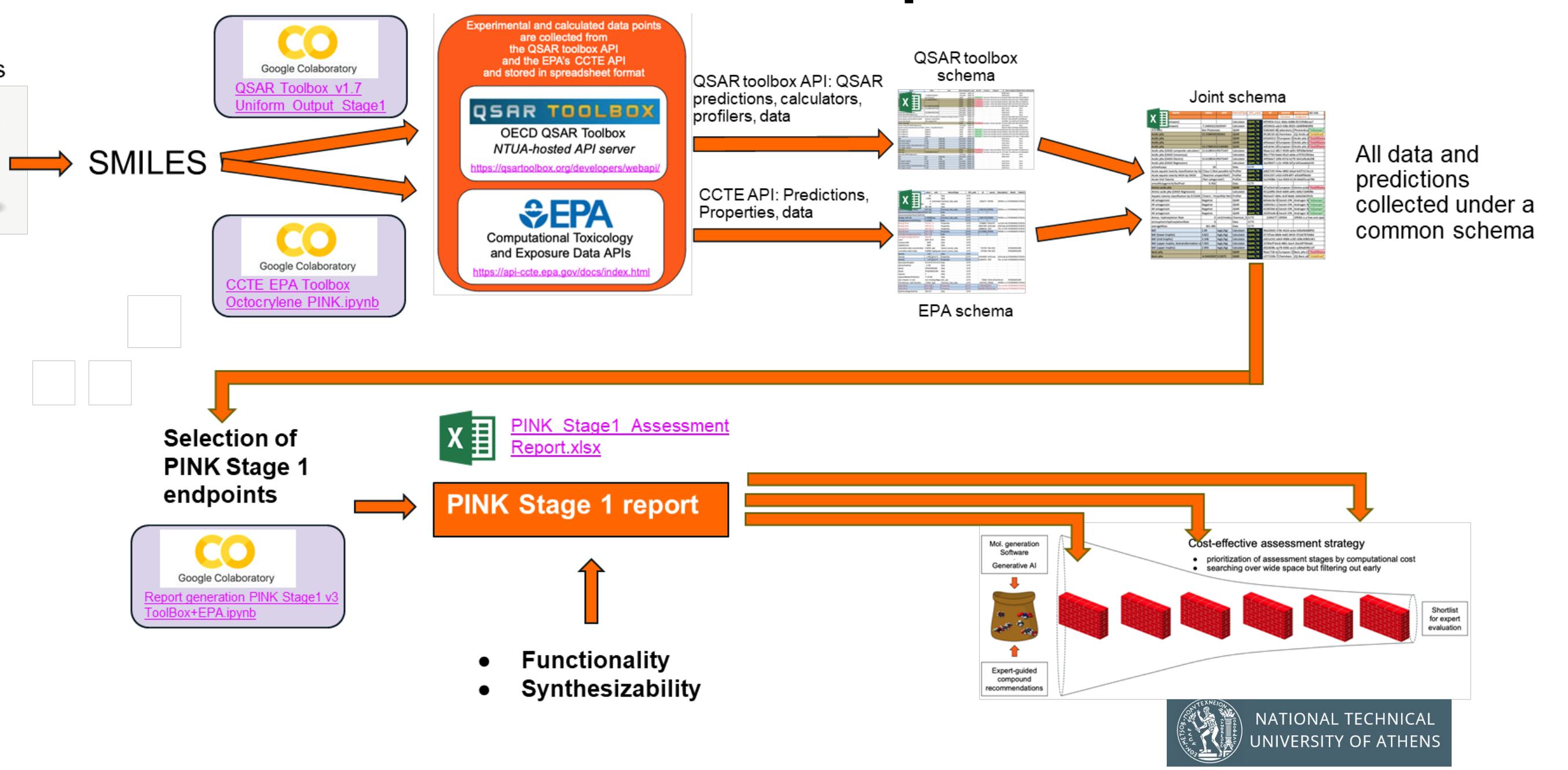
INTEGRATING COMPUTATIONAL MODELS AND BALANCING SSBD DIMENSIONS TO SATISFY THE INDUSTRY NEEDS FOR RESPONSIBLE INNOVATION ON ADVANCED MATERIALS AND CHEMICALS >PINK

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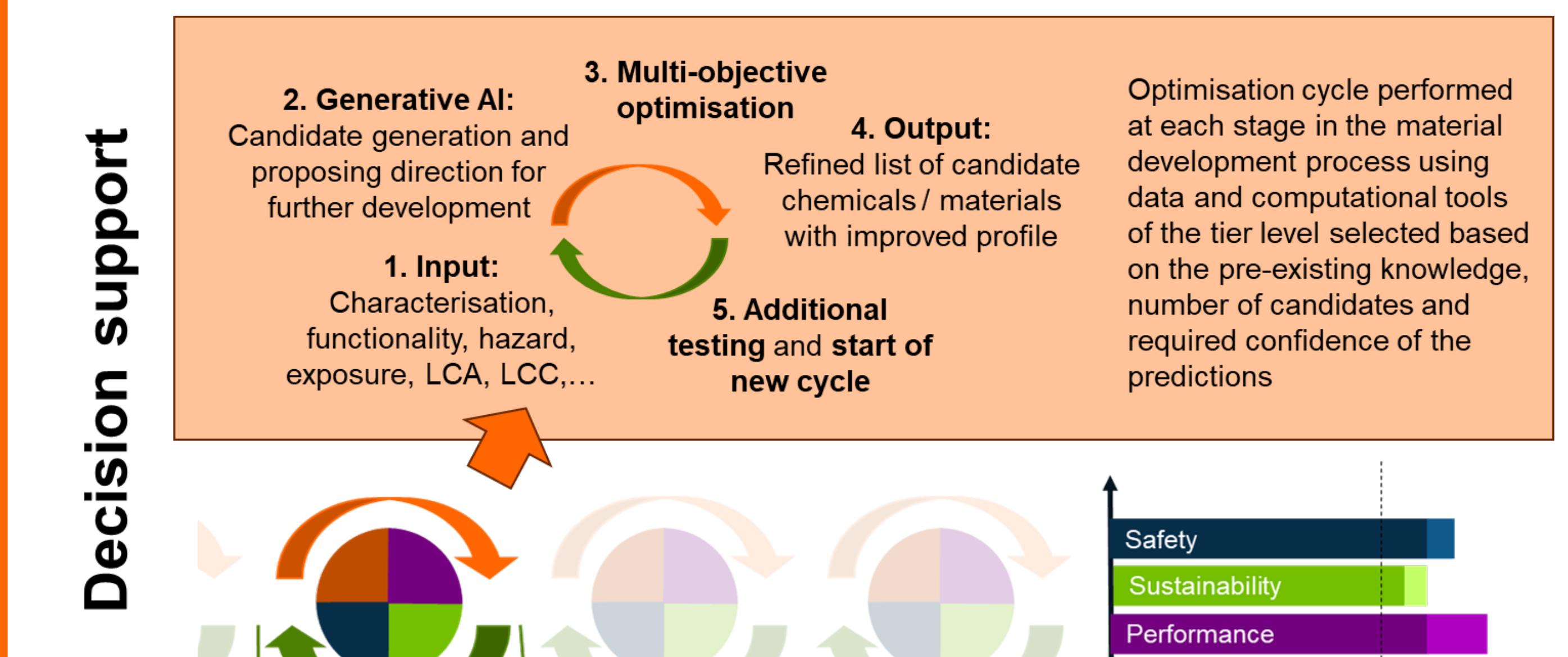
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Example for a data-driven chemicals SSbD step 1 optimization workflow



Decision support for (re-)design



2 Developmental case studies – 3 scenarios

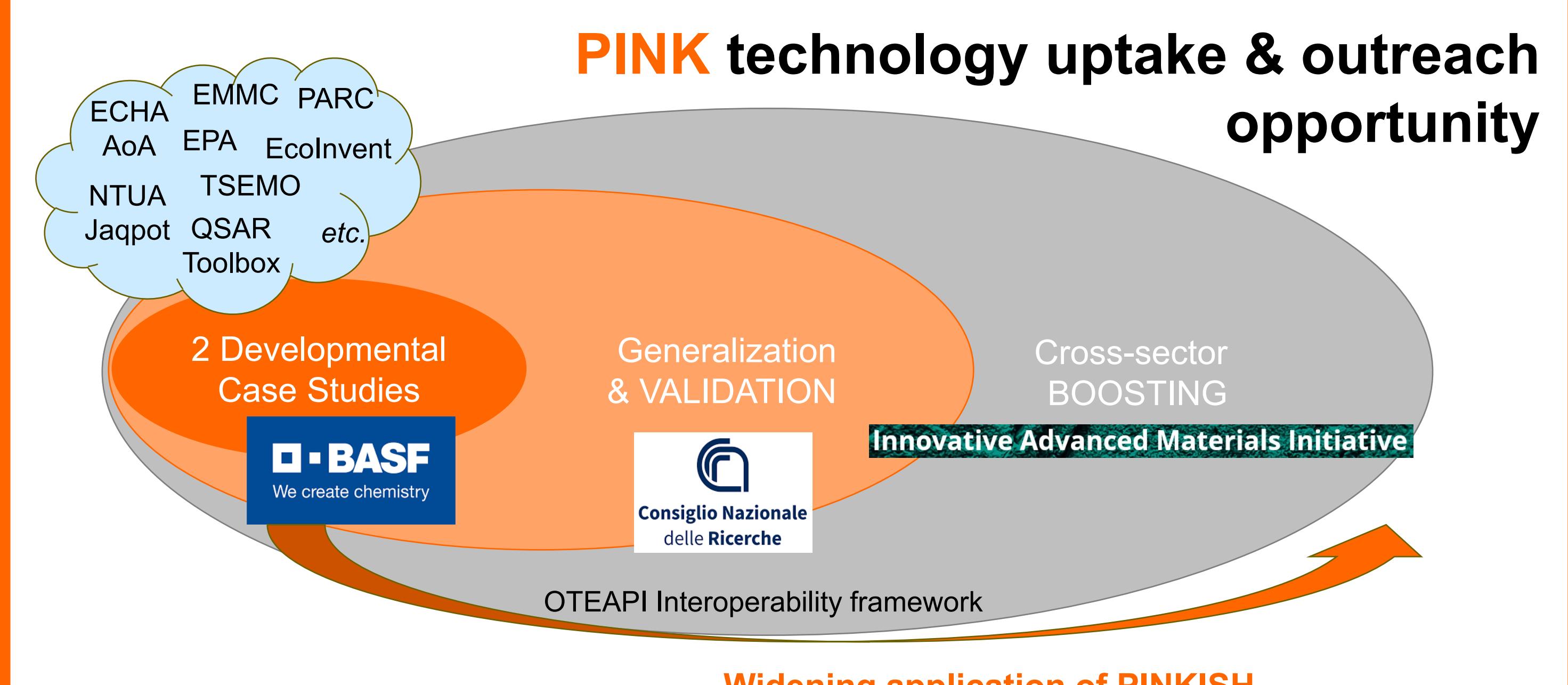
Scenario 1 - Business opportunity stage (Tier 1)
→ through inter-/extrapolation multiple candidates generated *in silico*; potential sustainability constraints determined by predictive modelling in parallel to functional performance testing/modelling;

Scenario 2 - Innovation development stage (Tier 2)
→ defined by one lead structure identified; some information is available (performance and partially safety and sustainability) with *in silico* tool-based modifications going on and sustainability criteria being evaluated;

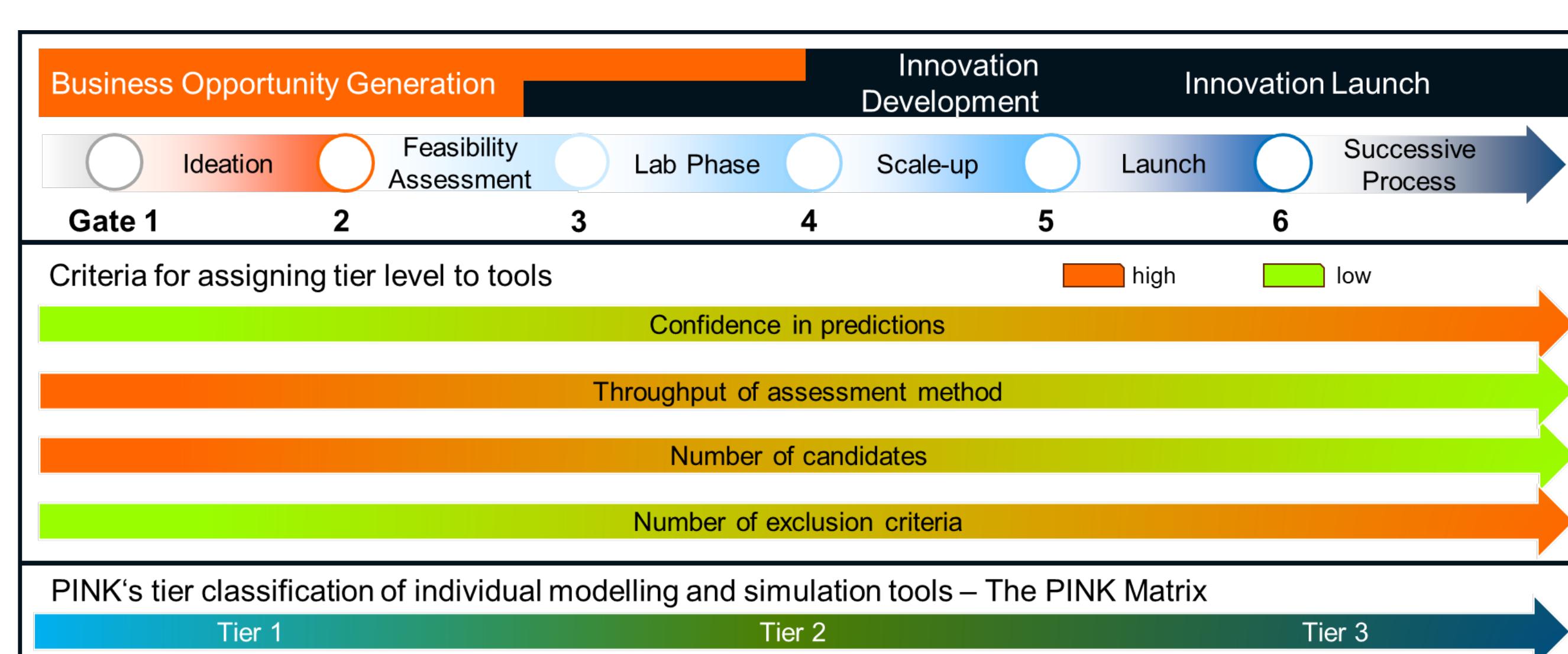
Scenario 3 - Material & innovation launch stages (Tier 3)

→ more data for several dimensions becomes available

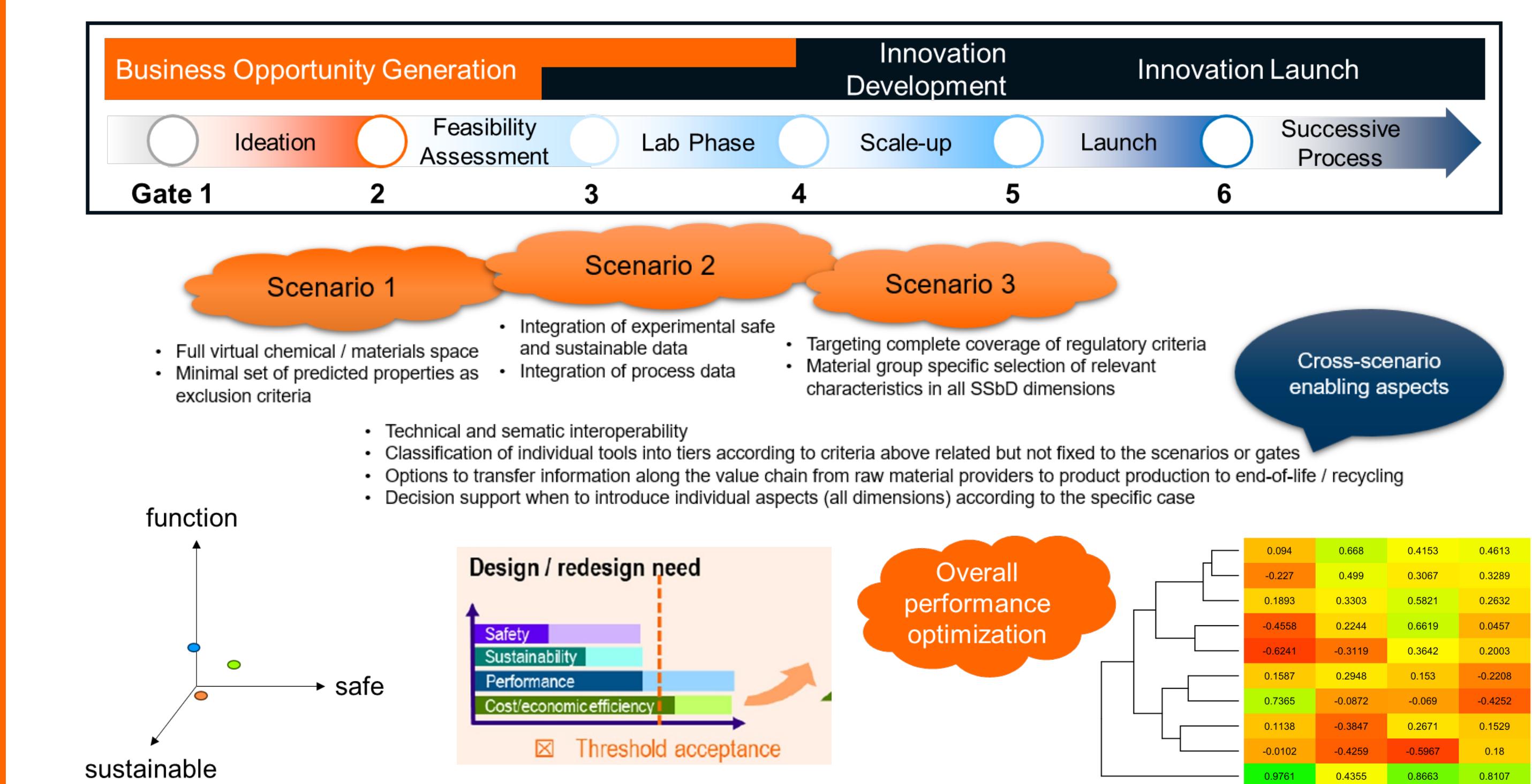
PINK technology uptake & outreach opportunity



PINK tiered approach



Re-design challenges @ different development stages



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