

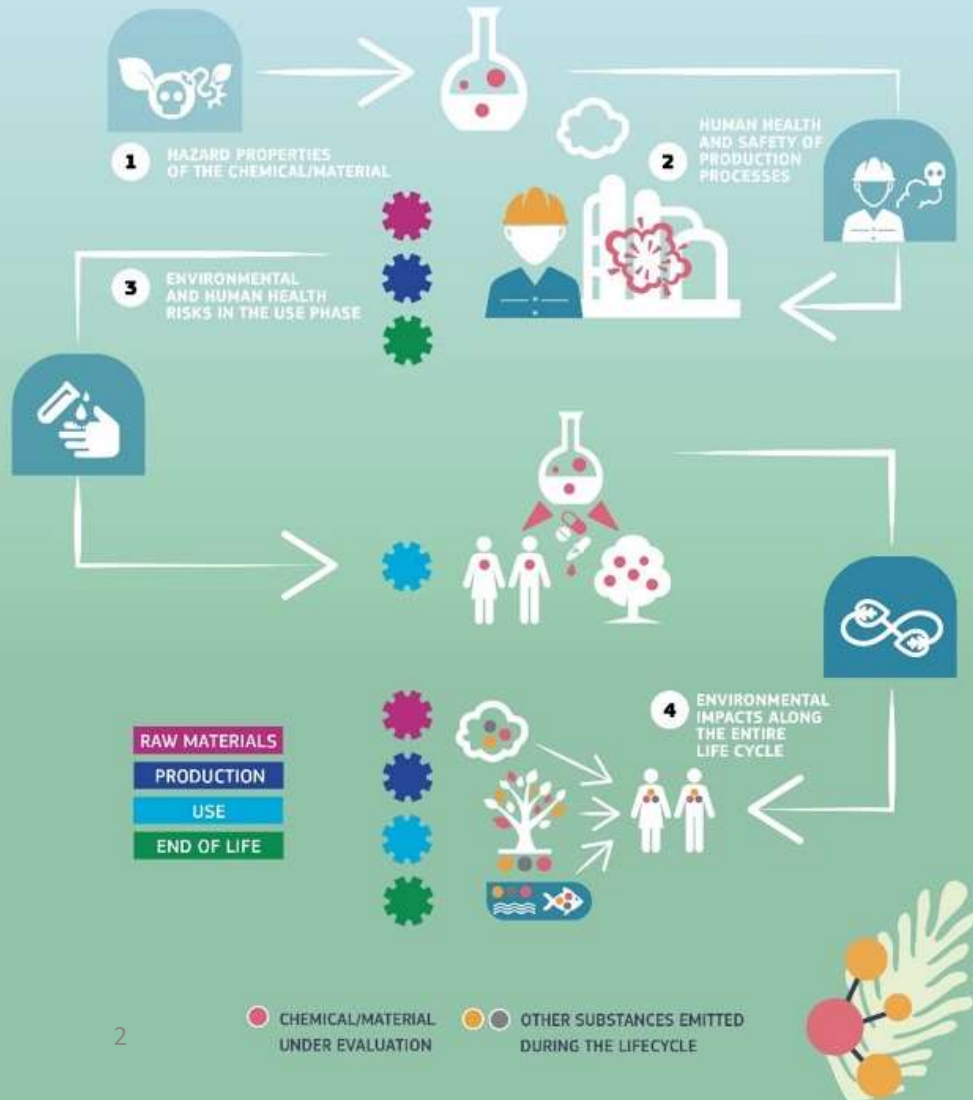


# LCA's alchemy challenge: assessing chemicals that do not exist

**André Bardow**  
ETH Zurich

86<sup>th</sup> LCA Discussion Forum: Safe- and Sustainable-by-Design

## Safety and sustainability assessment



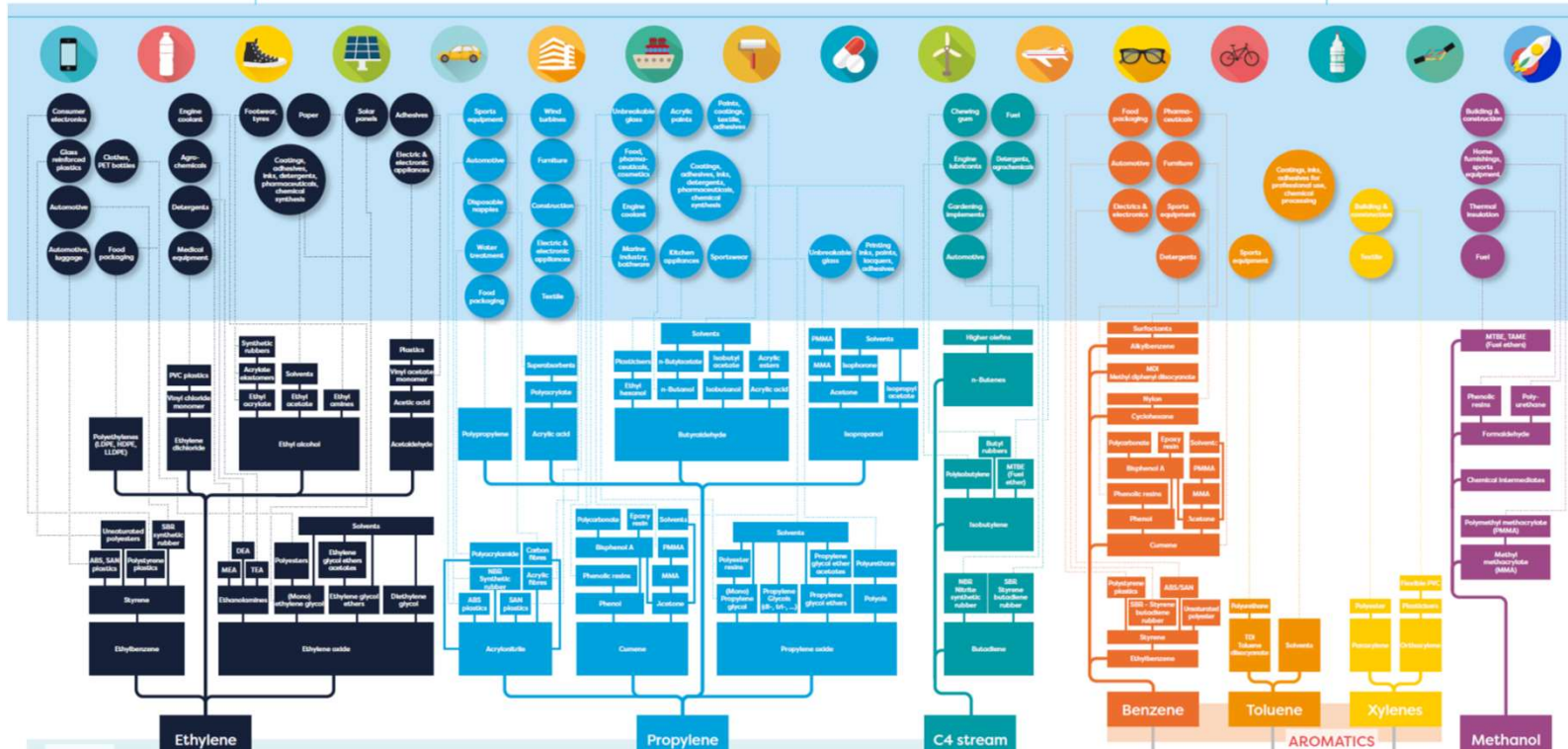
## SSbD framework:

to support the design and development of safe and sustainable chemicals and materials with research and innovation (R&I) activities

- The safety and sustainability assessment includes four steps:
  - **Step 1** - Hazard assessment of the chemical/material
  - **Step 2** - Human health and safety aspects in the chemical/material production and processing phase
  - **Step 3** - Human health and environmental aspects in the final application phase
  - **Step 4** - Environmental sustainability assessment along the entire chemical/material life cycle by means of an LCA

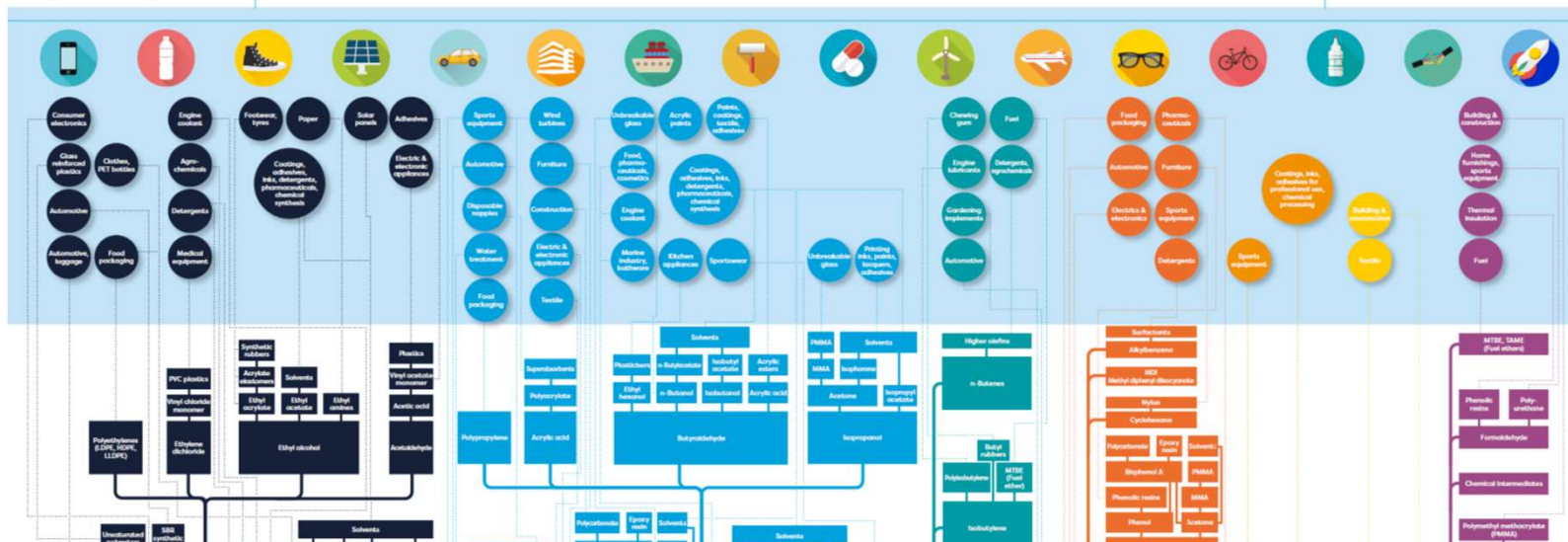


# LCA challenge for “design & development of chemicals”



- More than 30'000 products traded today
- LCA data bases contain few 100's of chemicals

# LCA challenge for “design & development of chemicals”



## Poor data and outdated methods sabotage the decarbonization efforts of the chemical industry

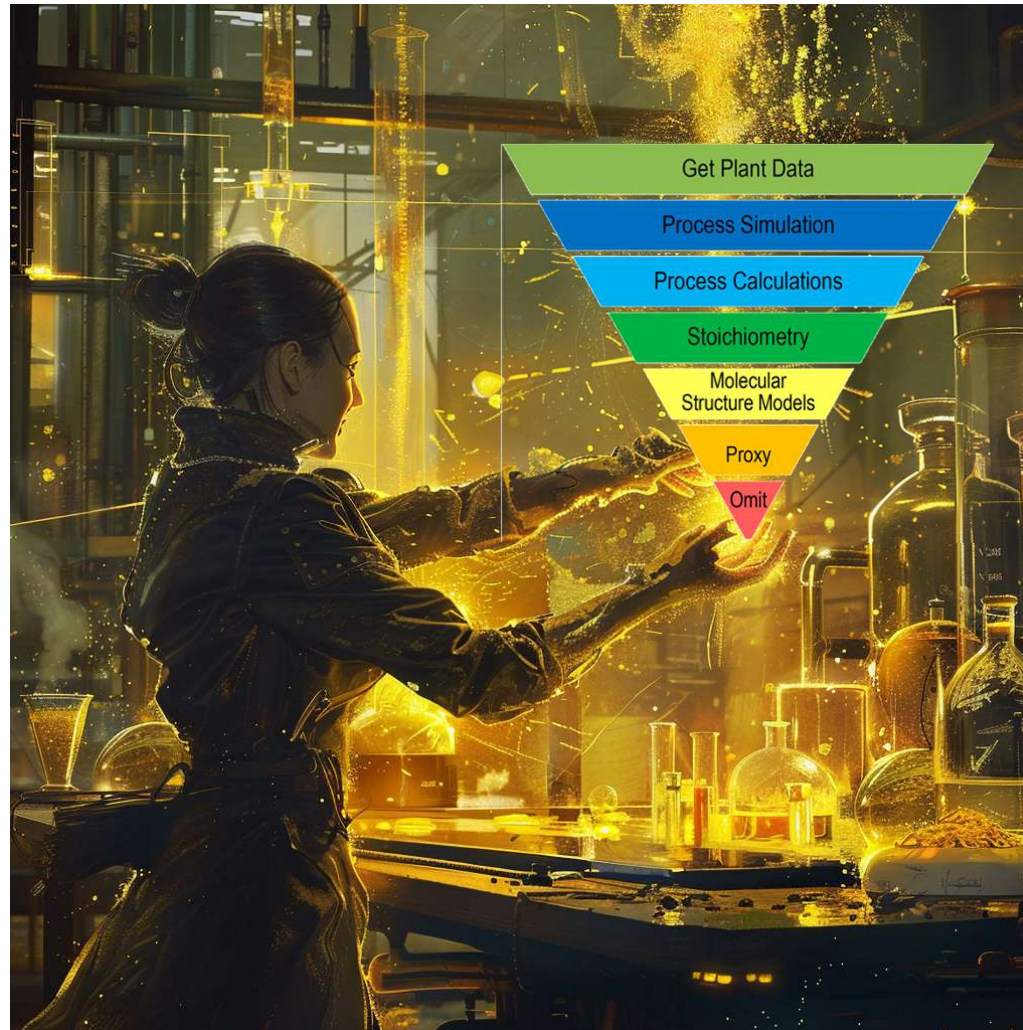
Christopher Oberschelp<sup>a,b\*</sup>, Stefanie Hellweg<sup>a,b</sup>, Eric Bradford<sup>a,b</sup>, Stephan Pfister<sup>a</sup>, Jing Huo<sup>a,b</sup>, and Zhanyun Wang<sup>a,b,c</sup>

<sup>a</sup>ETH Zürich, Institute of Environmental Engineering, John-von-Neumann-Weg 9, CH-8093 Zürich, Switzerland; <sup>b</sup>National Centre of Competence in Research (NCCR) Catalysis, ETH Zürich, CH-8093 Zürich, Switzerland; <sup>c</sup>Empa - Swiss Federal Laboratories for Materials Science and Technology, Technology and Society Laboratory, Lerchenfeldstrasse 5, CH-9014 St. Gallen, Switzerland; \* Correspondence: [cobersch@ethz.ch](mailto:cobersch@ethz.ch)

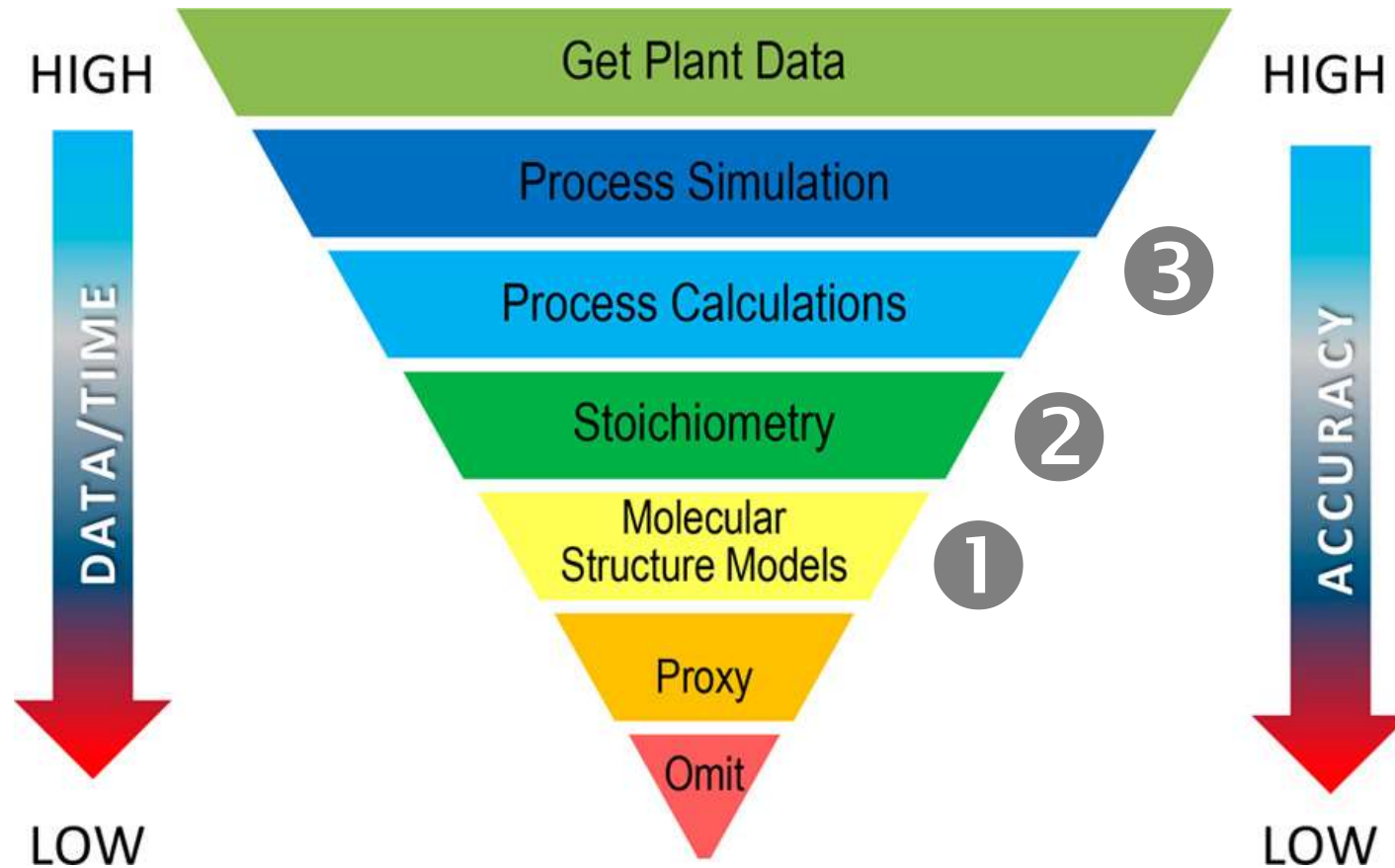
<https://doi.org/10.26434/chemrxiv-2023-8c86t>



# LCA's alchemy challenge: how to create data from nothing ?

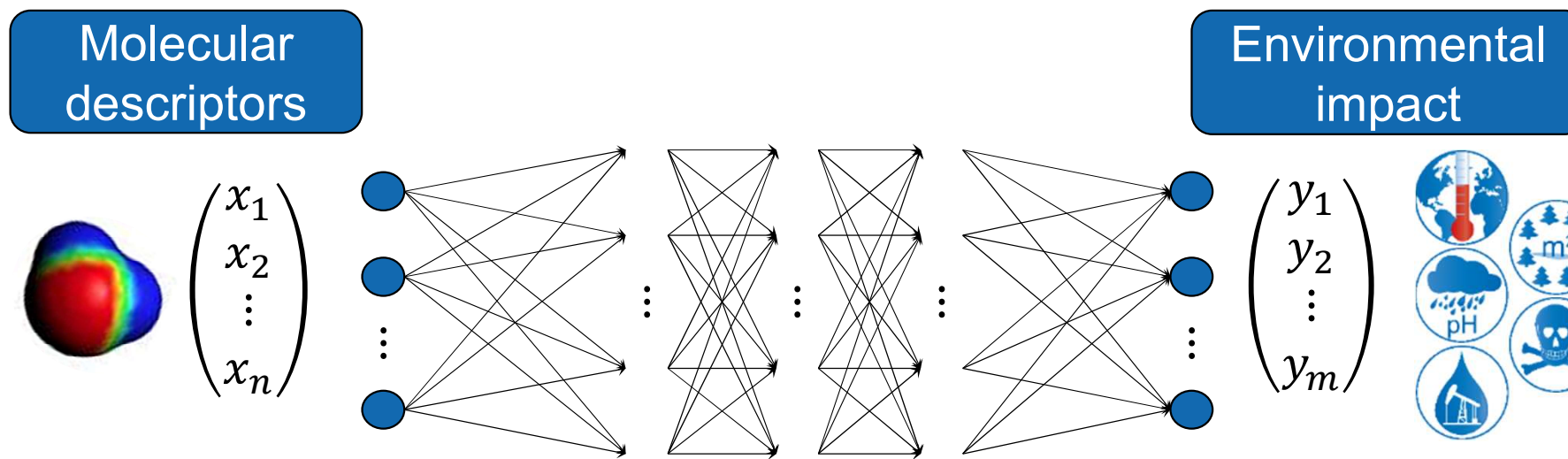


# LCA's alchemy challenge: how to create data from nothing ?



Parvatker & Eckelman, *ACS Sustainable Chem. Eng.* 2019, 7, 1, 350-367

# Molecular structure models for LCA



*Environ. Sci. Technol.* **2008**, *42*, 6717–6722

## Molecular-Structure-Based Models of Chemical Inventories using Neural Networks

GREGOR WERNET,\* STEFANIE HELLWEG, ULRICH FISCHER, STAVROS PAPADOKONSTANTAKIS, AND KONRAD HUNGERBÜHLER

Swiss Federal Institute of Technology, Safety and Environmental Technology Group, HCI G143, Wolfgang-Pauli-Strasse 10, CH-8093 Zurich.

Chemical synthesis specialized equipment solvents or catalysts or steam, and unique chemicals such as products difficult to acquire. quantities than most usually more complex are generally produced alongside with measurements of use—difficult. In addition, secrets, and chemical data publicly available. For these reasons,

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**Sustainable**  
Chemistry & Engineering

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Research Article

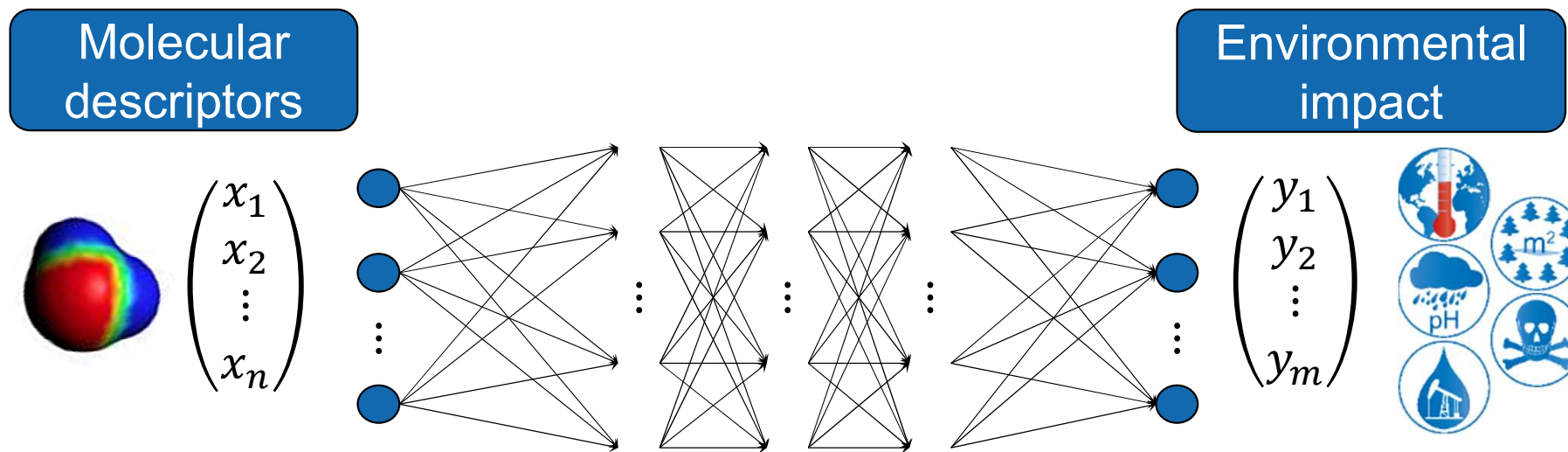
## Enhanced Deep-Learning Model for Carbon Footprints of Chemicals

Dachuan Zhang,\* Zhanyun Wang, Christopher Oberschelp, Eric Bradford, and Stefanie Hellweg

Cite This: <https://doi.org/10.1021/acscuschemeng.3c07038>

Read Online

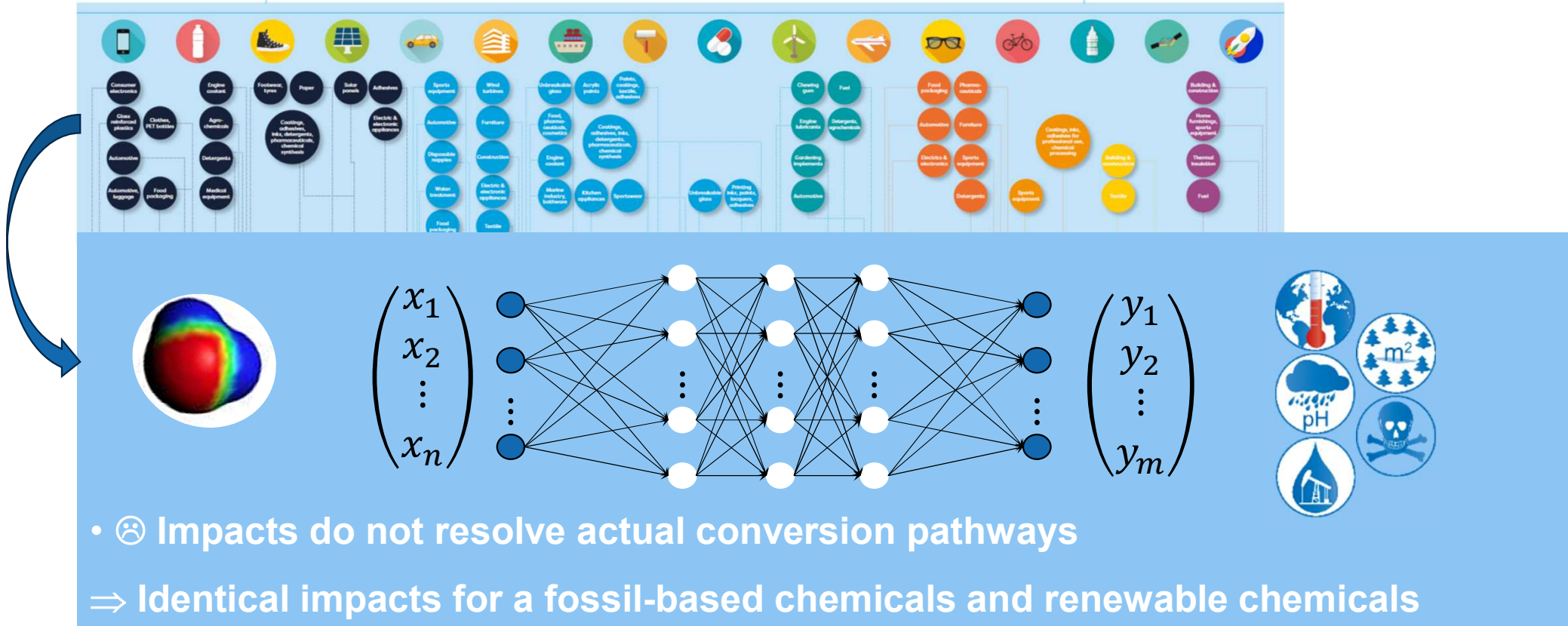
# Molecular structure models for LCA



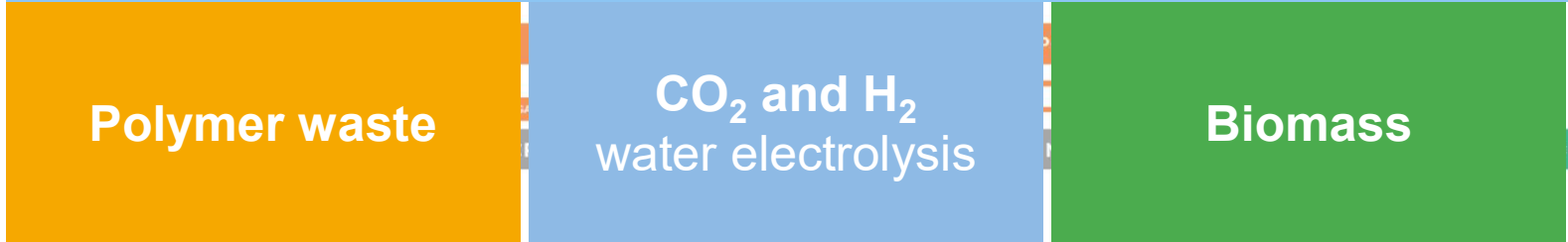
- 😊 Input: Molecular information starting from name only (SMILES)
- 😊 Improved estimation in FineChem 2: RMSE down by 55% to 2.9 kg<sub>CO2-equiv</sub>/kg
- 😞 Impacts do not resolve actual conversion pathways



# LCA challenge for “design & development of chemicals”



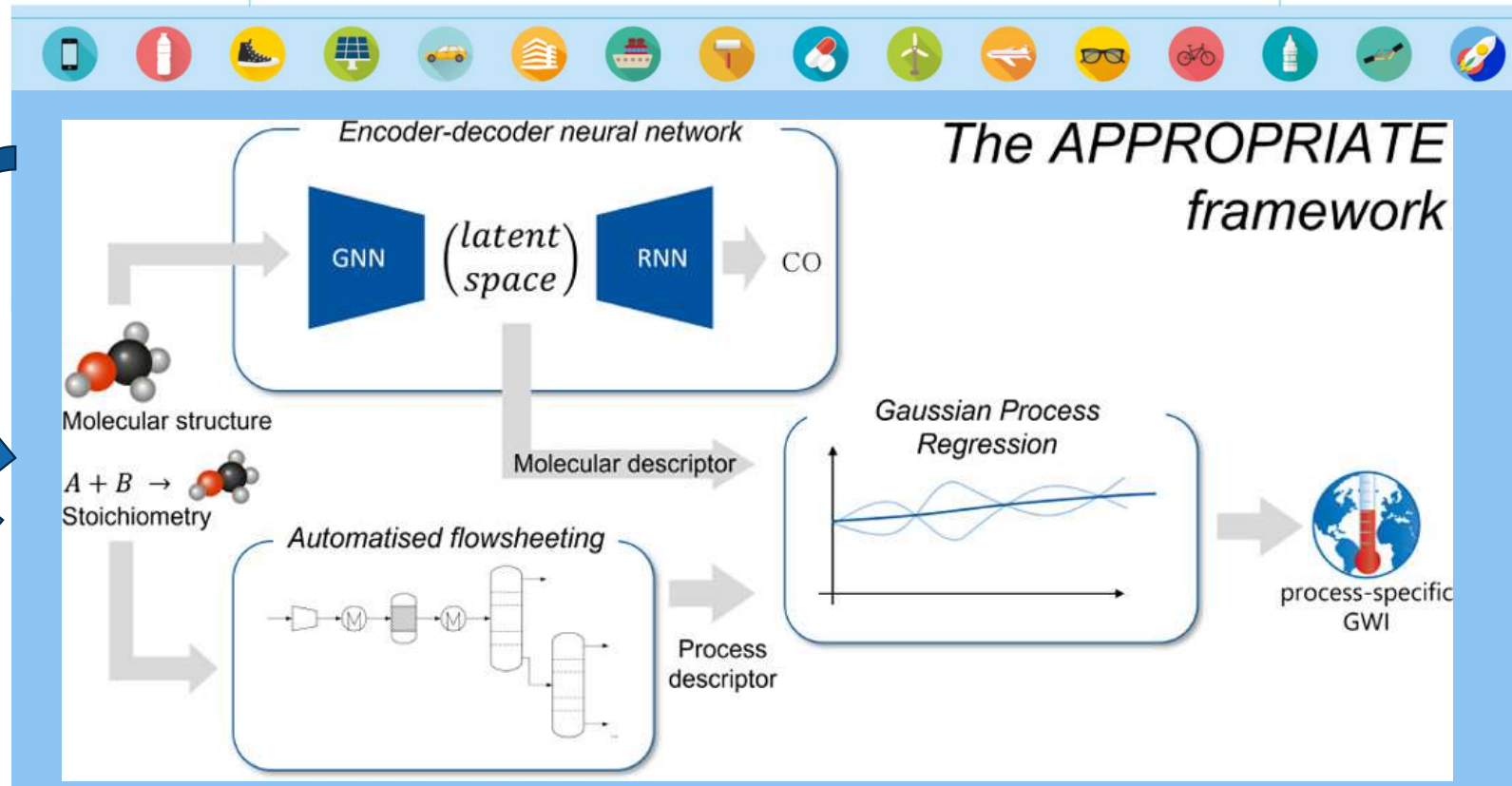
- ⊖ Impacts do not resolve actual conversion pathways
- ⇒ Identical impacts for a fossil-based chemicals and renewable chemicals



# PROcess-Specific, PRedictive Impact Assessment



Johanna Kleinekorte



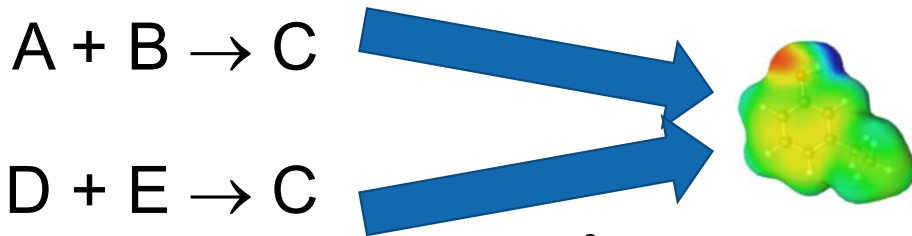
Polymer waste

CO<sub>2</sub> and H<sub>2</sub>  
water electrolysis

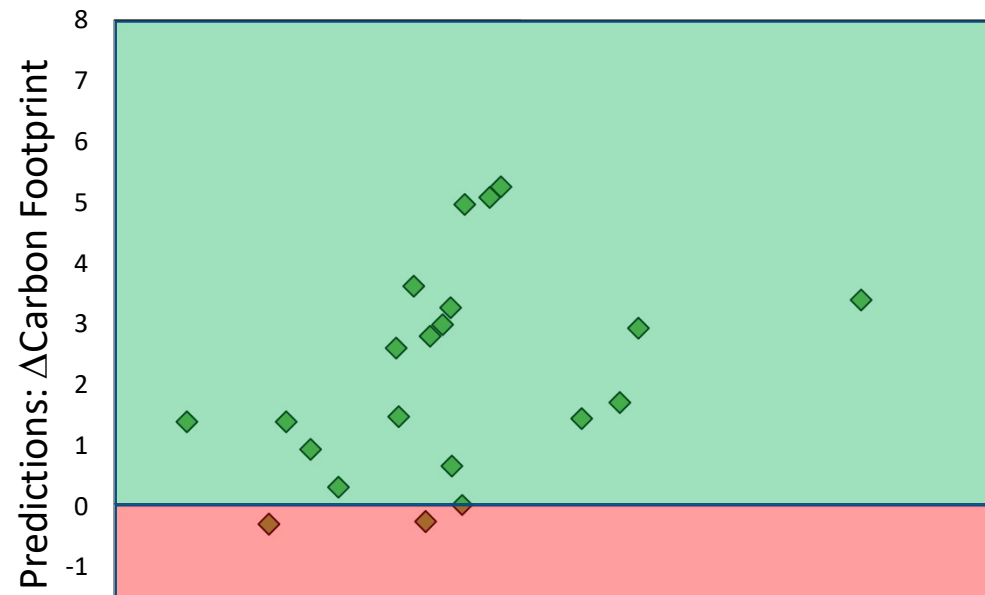
Biomass

Kleinekorte et al., ACS Sustainable Chem. Eng. 2023, 11, 25, 9303-9319

# Predictive LCA for process alternatives



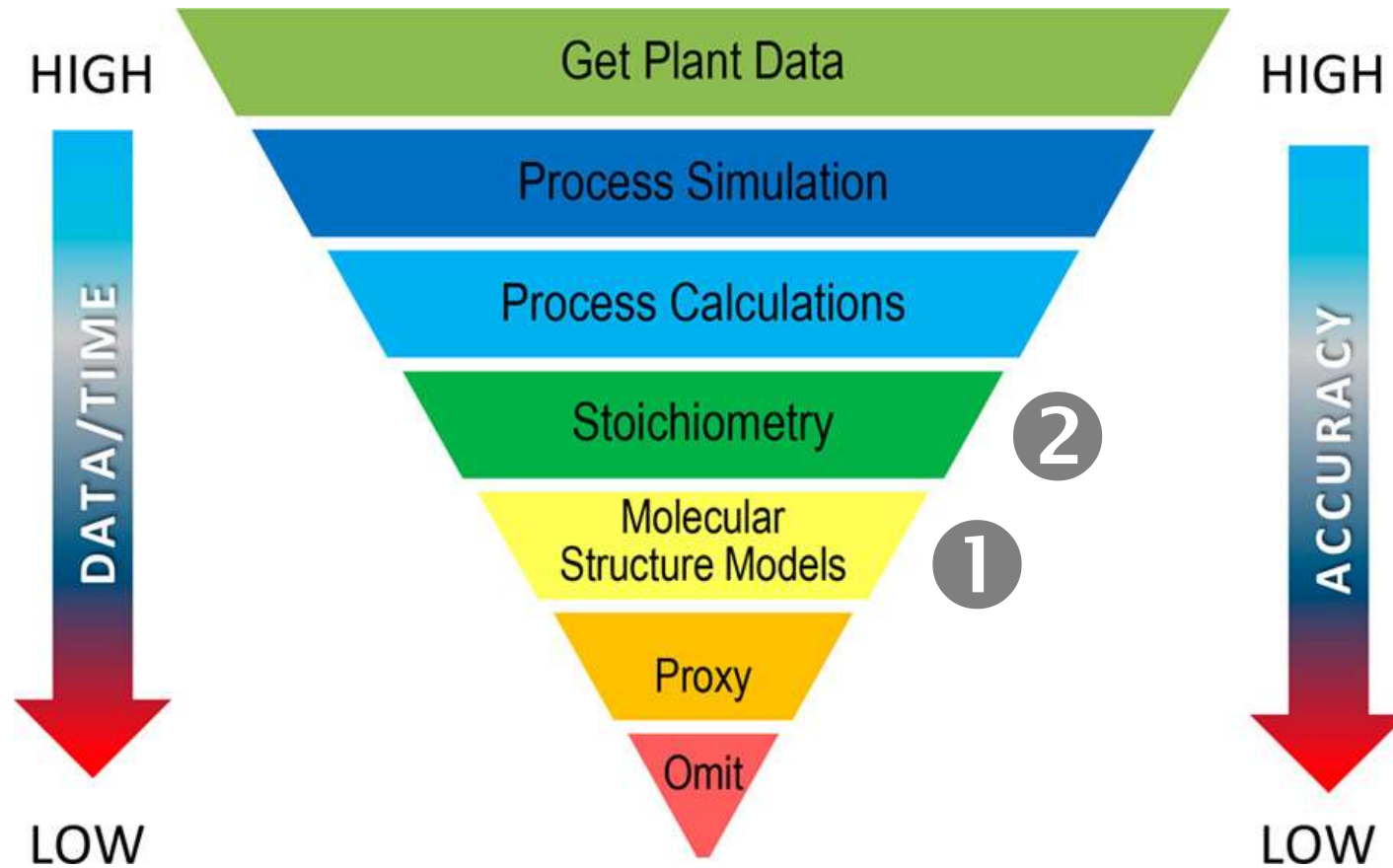
Johanna  
Kleinekorte



Model identifies 84% of low-carbon process correctly



# LCA's alchemy challenge: how to create data from nothing ?

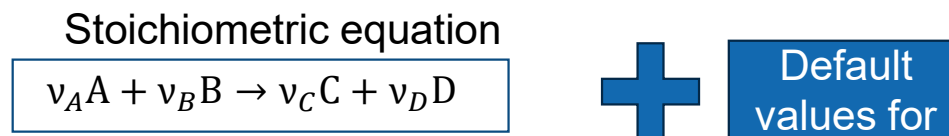


Parvatker & Eckelman, *ACS Sustainable Chem. Eng.* 2019, 7, 1, 350-367

# Predictive LCA today: Stoichiometry

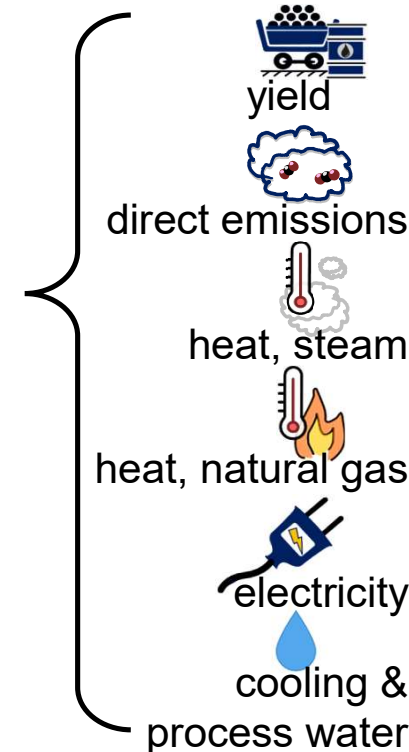
## Stoichiometry-based assessment

- Impacts for chemicals often dominated by reactants
- Common heuristic (e.g., ecoinvent):

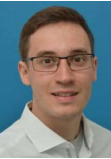


**Benchmarking**

**Stoichiometry-based assessment ?**

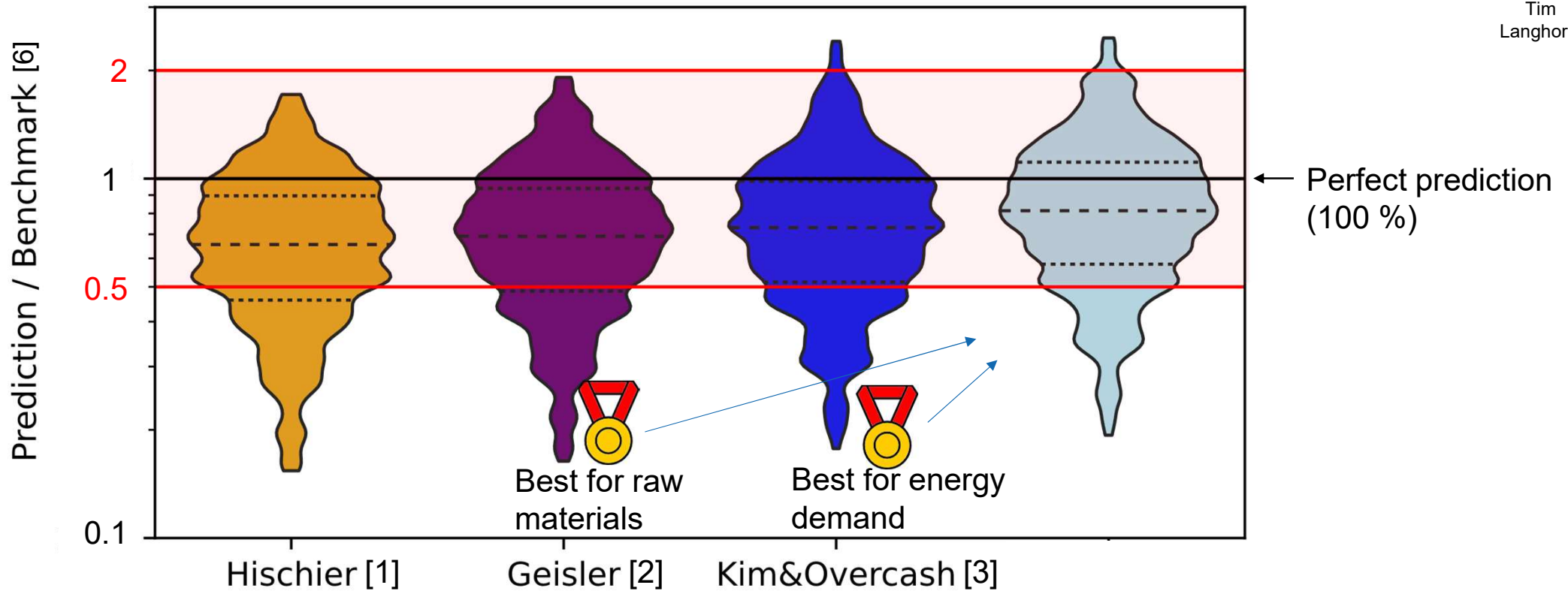


# Benchmarking stoichiometry-based assessment



Tim  
Langhorst

## Global Warming Potential



[1] Hischer R, Hellweg S, Capello C, Primas A.. *Int J LCA*. 2005. doi:10.1065/lca2004.10.181.7.

[2] Geisler G, Hofstetter TB, Hungerbühler K.. *Int J LCA*. 2004. doi:10.1007/BF02978569.

[3] Kim S, Overcash M. *J. Chem. Technol. Biotechnol.* 2003. doi:10.1002/jctb.821.

[6] Langhorst T, Winter B, Roskosch D, Bardow A.. *ACS Sus Chem Eng*. 2023. doi:10.1021/acssuschemeng.2c07624

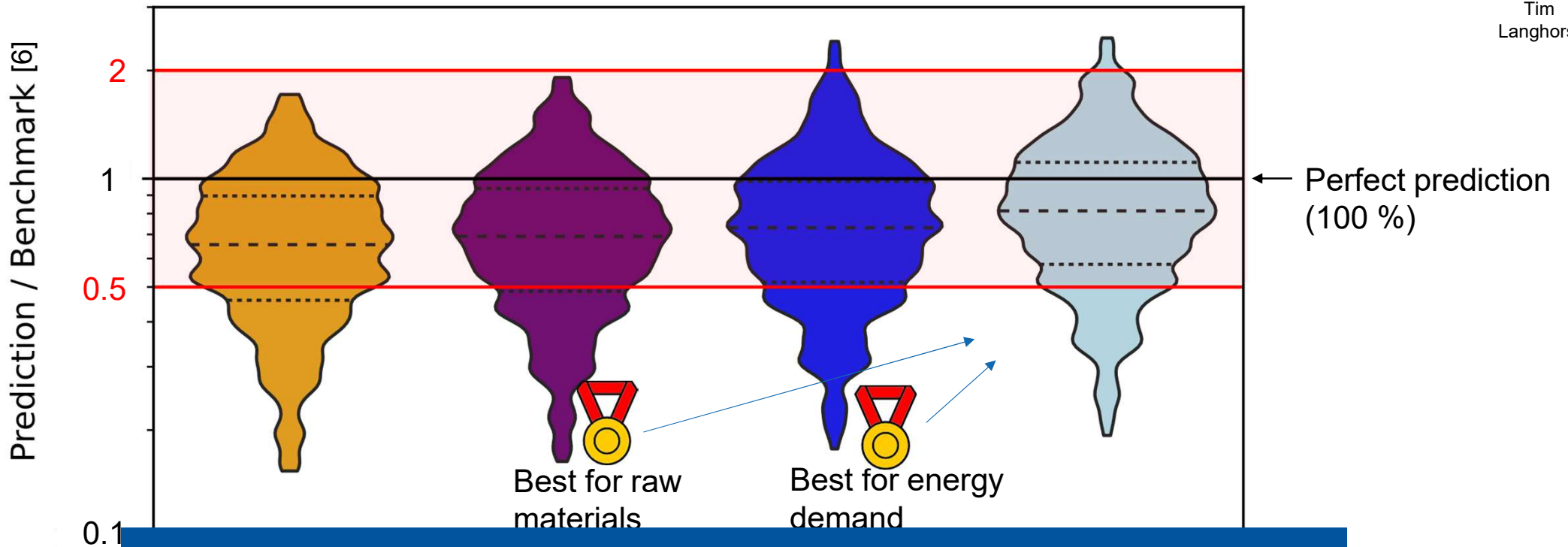


# Benchmarking stoichiometry-based assessment



Tim  
Langhorst

## Global Warming Potential

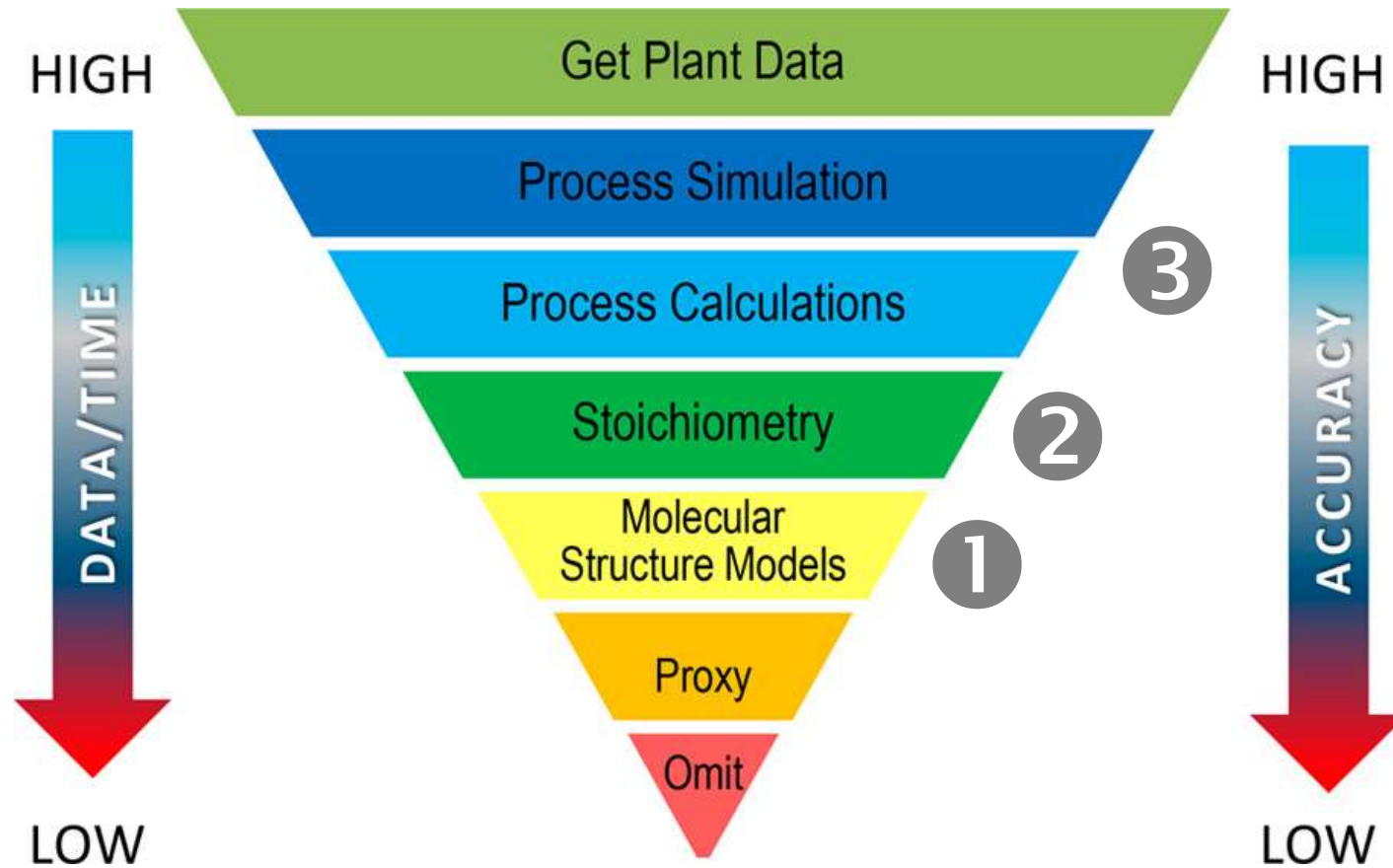


**Quality of stoichiometric-based LCA estimation corresponds to economic estimation methods**

2004.10.181.7.  
2978569.  
1.

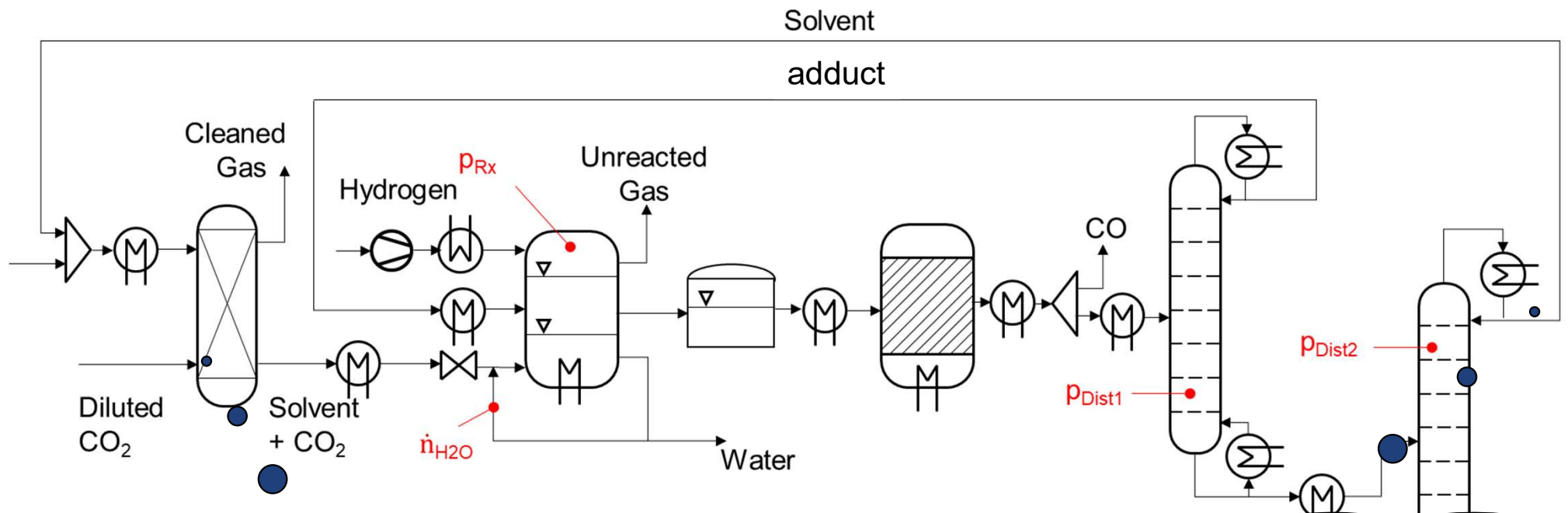
[6] Langhorst T, Winter B, Roskosch D, Bardow A.. ACS Sus Chem Eng. 2023. doi: 10.1021/acssuschemeng.2c07624

# LCA's alchemy challenge: how to create data from nothing ?



Parvatker & Eckelman, *ACS Sustainable Chem. Eng.* 2019, 7, 1, 350-367

# Automated Flowsheet: Integrated CO<sub>2</sub> capture & conversion



**The optimal unit operations?**

**The optimal configuration?**

Absorption

Synthesis

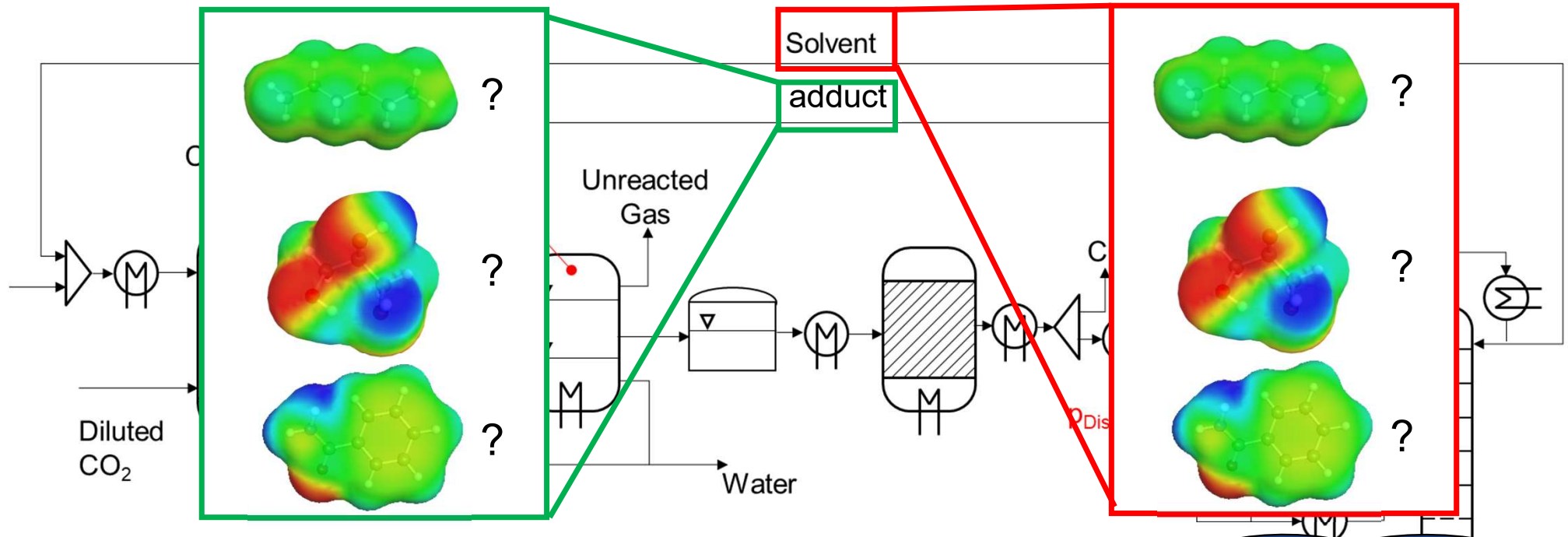
Storage

Reforming

Distillation

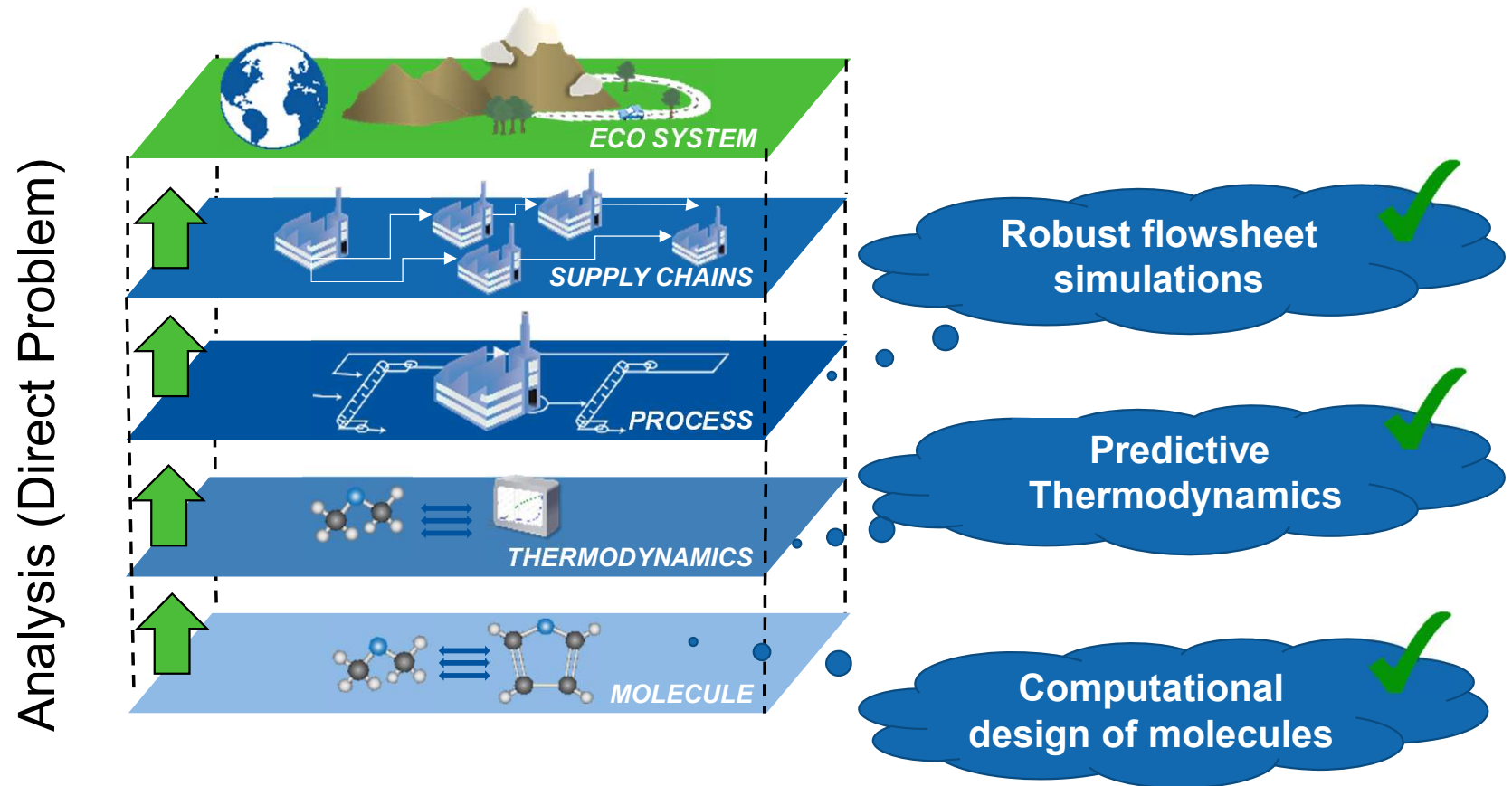


# Automated Flowsheet: Integrated CO<sub>2</sub> capture & conversion

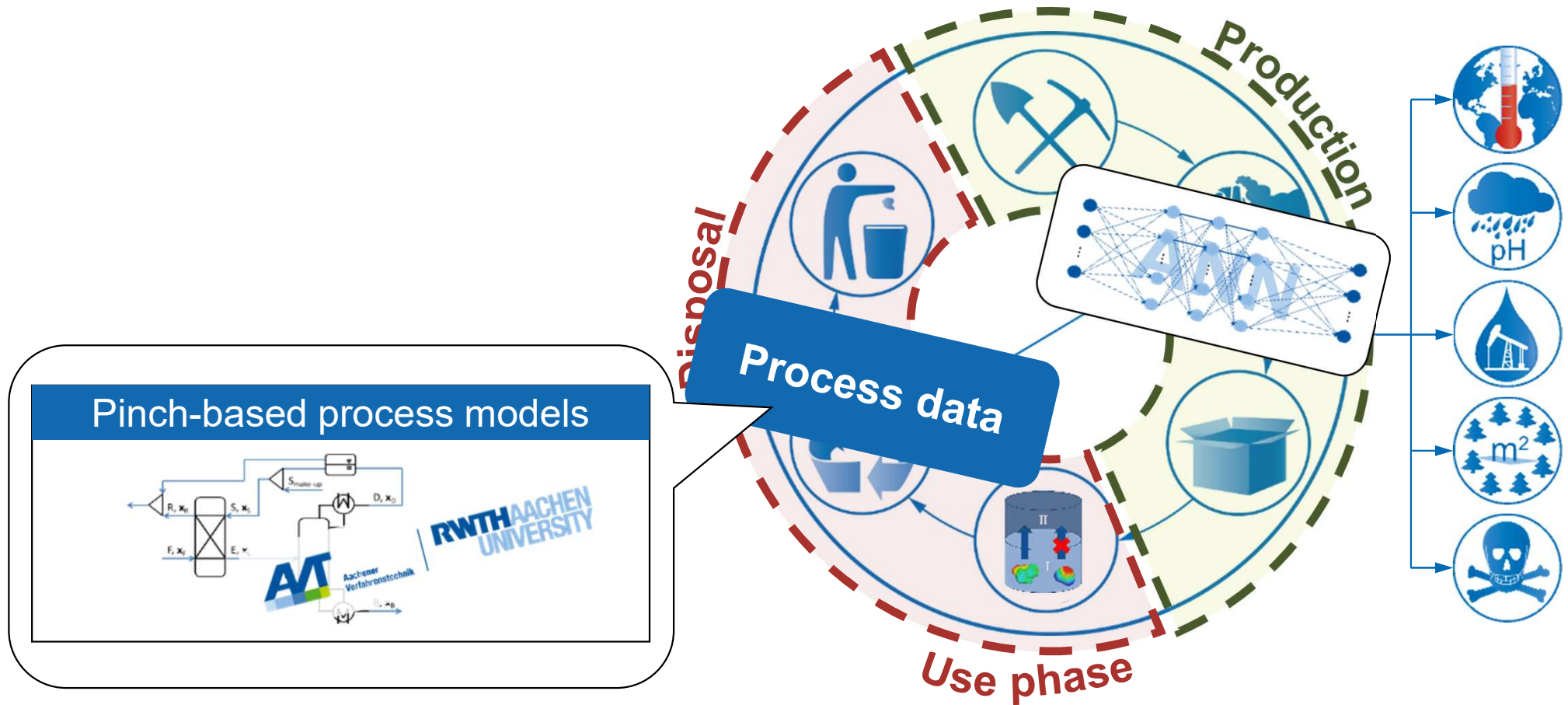


Unlimited degrees of freedom in process design  
⇒ Impact on impacts

# From molecules to sustainable life cycles



# Predictive process-level LCA





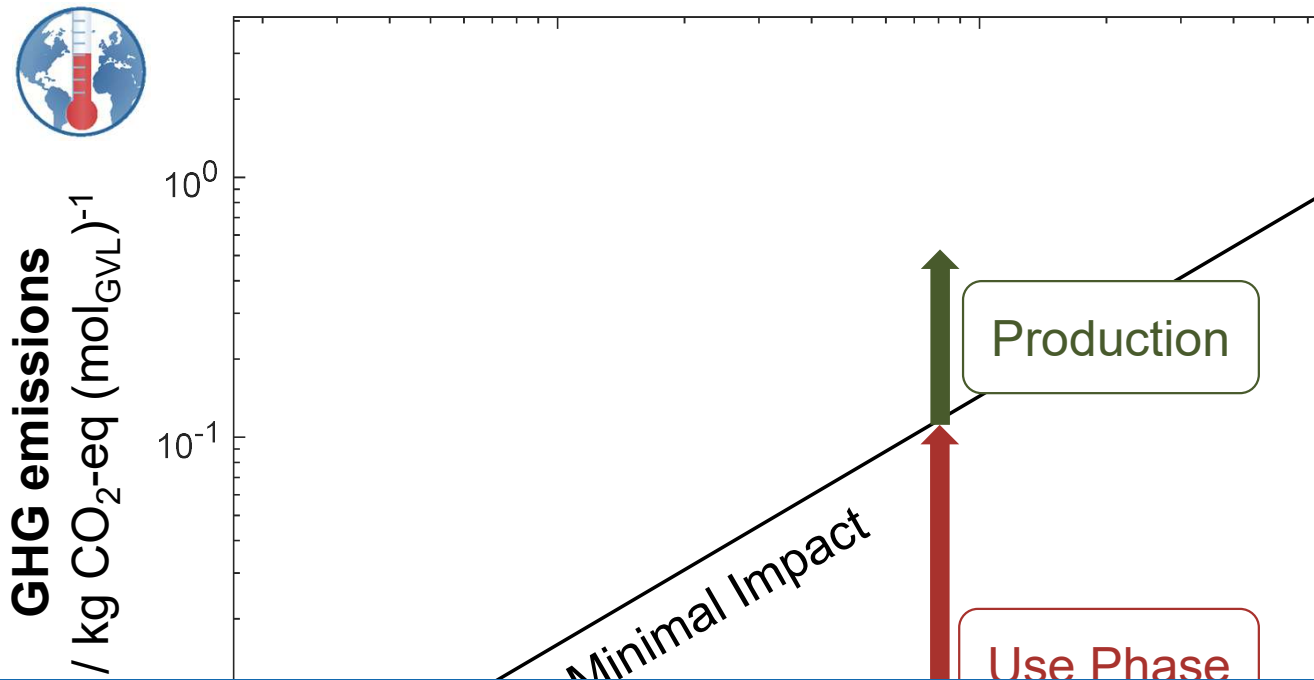
# Predictive process-level LCA



Lorenz  
Fleitmann

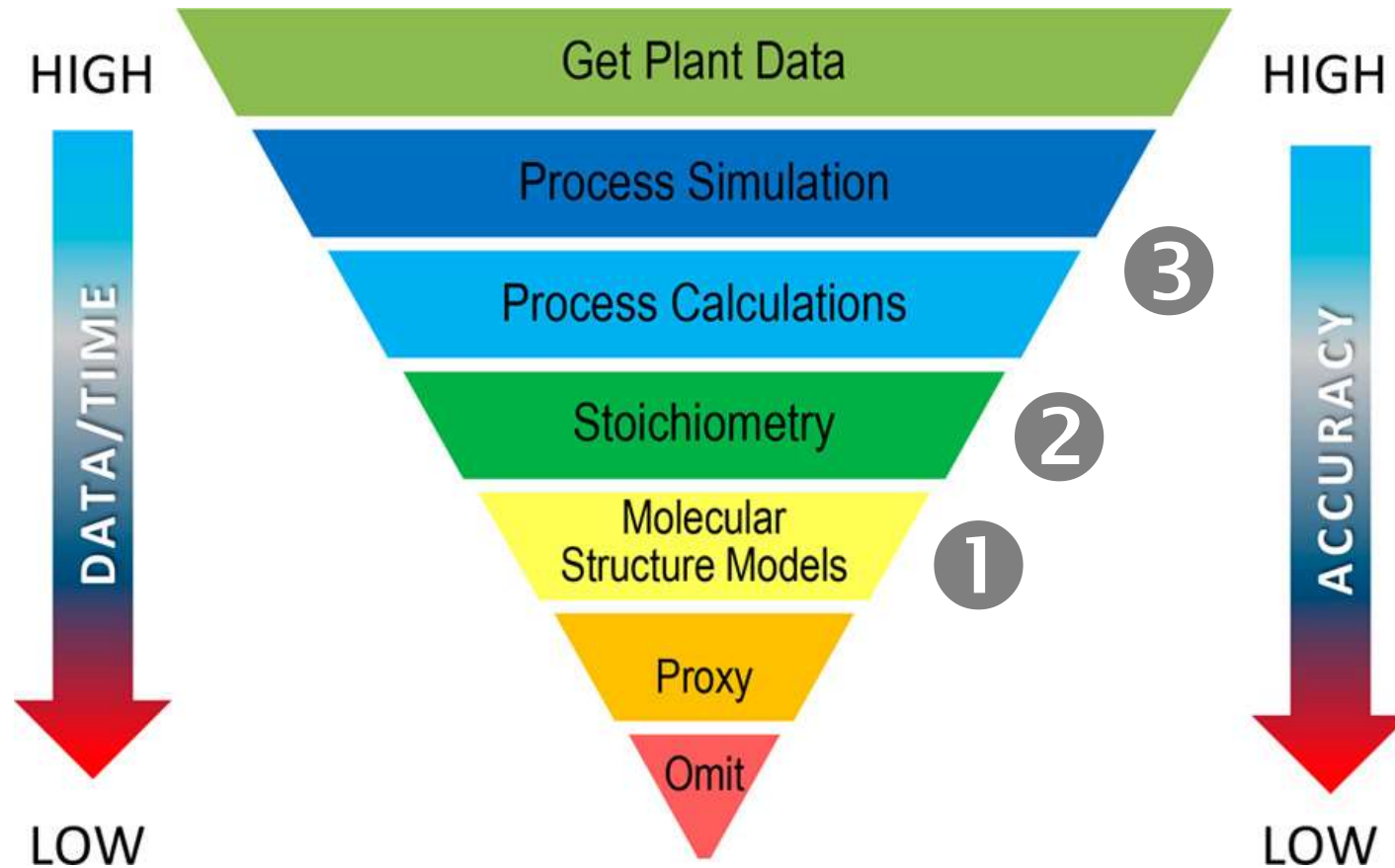


Johanna  
Kleinekorte



Toolbox established  
to predict LCA data for early-stage technology

# LCA's alchemy challenge: how to create data from nothing ?

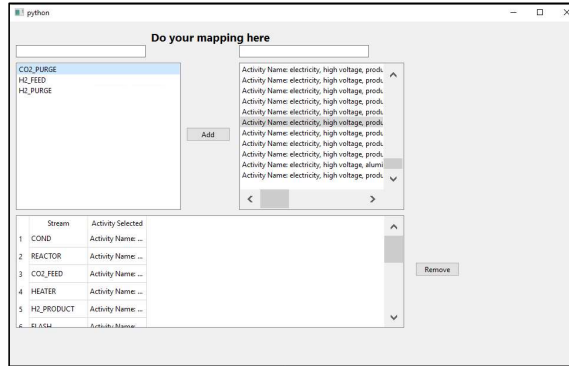


Parvatker & Eckelman, *ACS Sustainable Chem. Eng.* 2019, 7, 1, 350-367

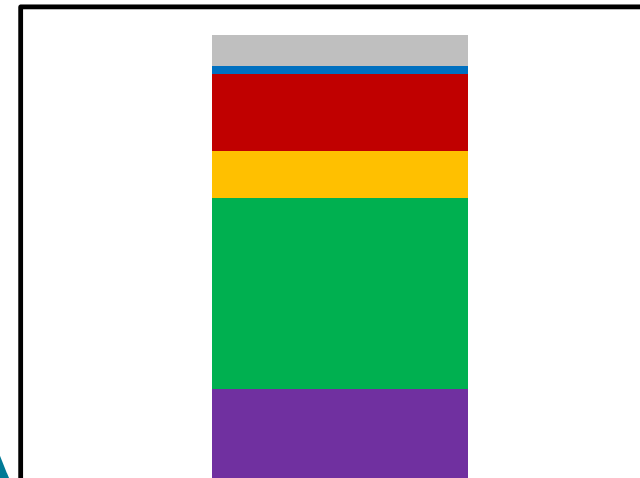
# Automated Life Cycle Assessment – automated workflow



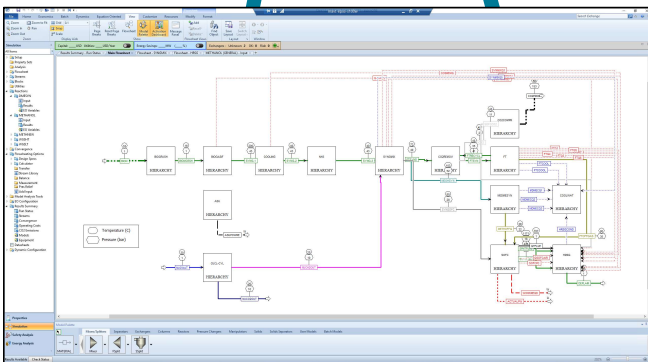
Lukas Spiekermann



Climate Change Impact  
in  $\text{kg}_{\text{CO2eq}}/\text{kg}_{\text{Product}}$

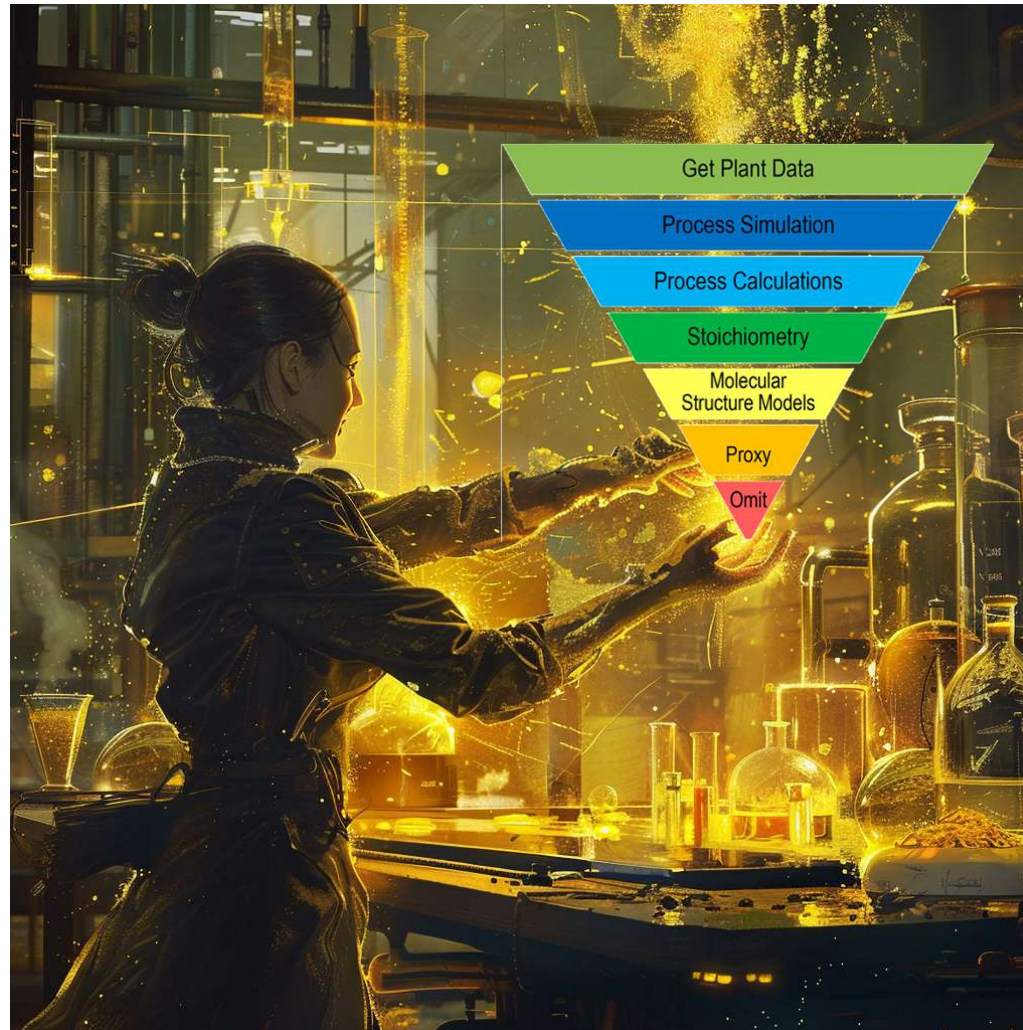


- Waste
- Cooling
- Heat
- Electricity
- Feedstock B
- Feedstock A

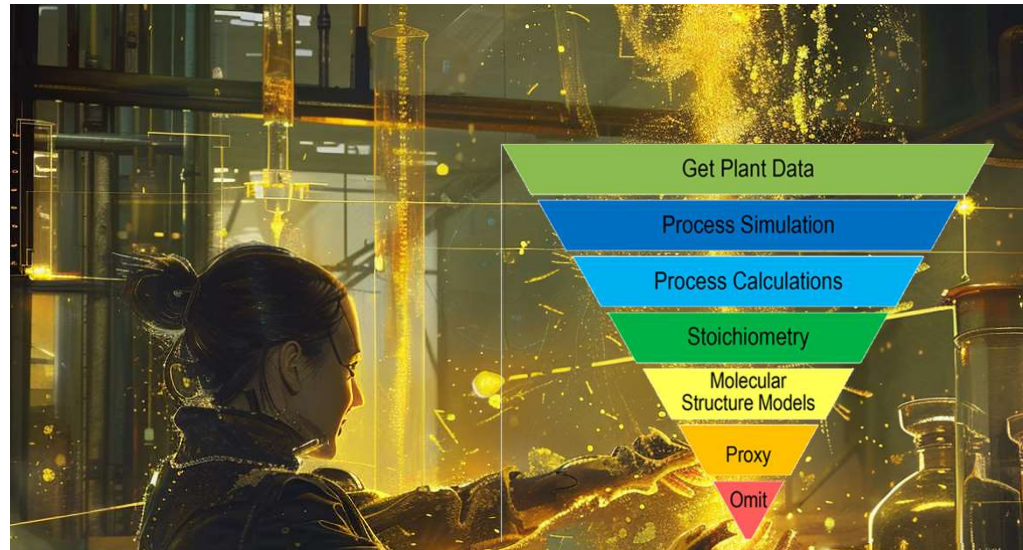




# LCA's alchemy challenge: how to create data from nothing ?



LCA's alchemy challenge: how to create data from nothing ?



*Good*

*up*

*Support*

# ~~Poor data and outdated methods sabotage the decarbonization efforts of the chemical industry~~

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<sup>a</sup>ETH Zürich, Institute of Environmental Engineering, John-von-Neumann-Weg 9, CH-8093 Zürich, Switzerland; <sup>b</sup>National Centre of Competence in Research (NCCR) Catalysis, ETH Zürich, CH-8093 Zürich, Switzerland; <sup>c</sup>Empa - Swiss Federal Laboratories for Materials Science and Technology, Technology and Society Laboratory, Lerchenfeldstrasse 5, CH-9014 St. Gallen, Switzerland; \* Correspondence: [coersch@ethz.ch](mailto:coersch@ethz.ch)

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