

AI-guided CO₂ conversion

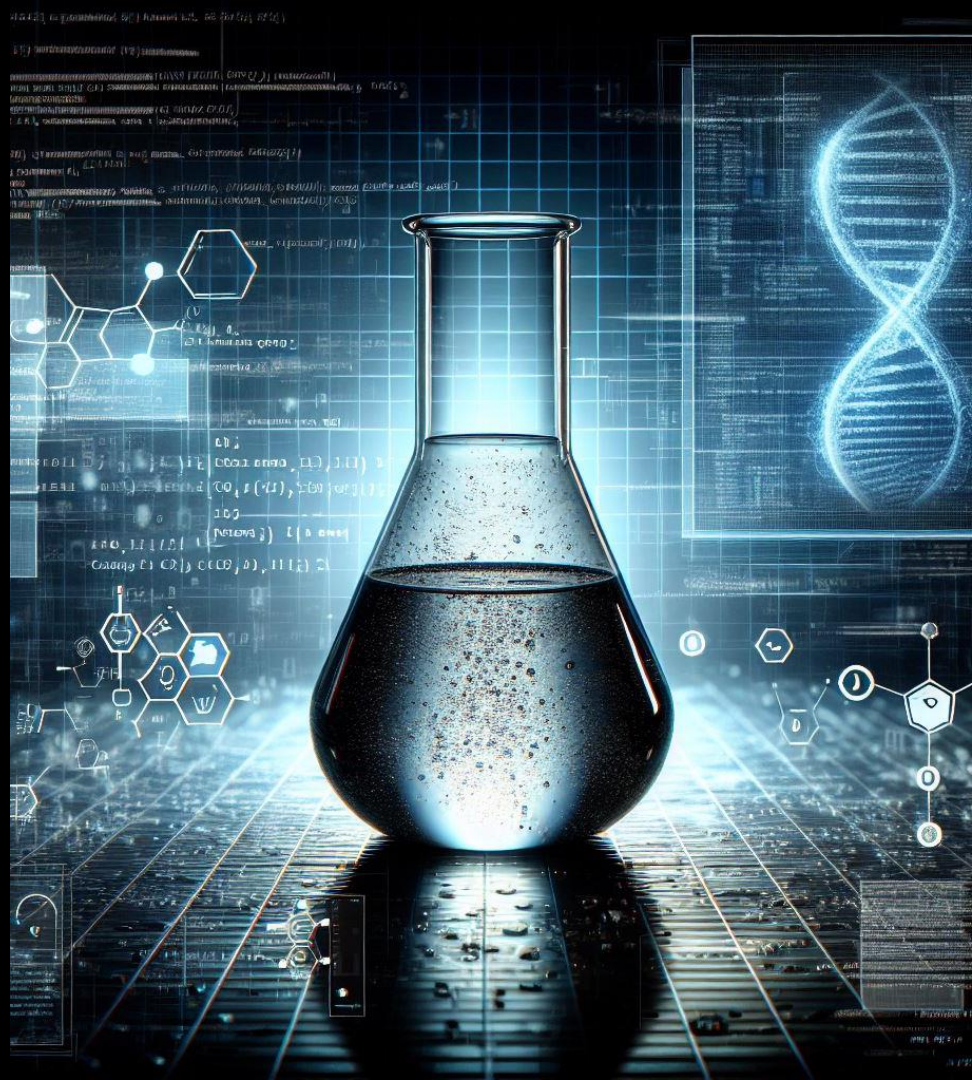
An AKA/RRF project

Prof. Annukka Santasalo-Aarnio
11.12.2024, Pikku-Finlandia

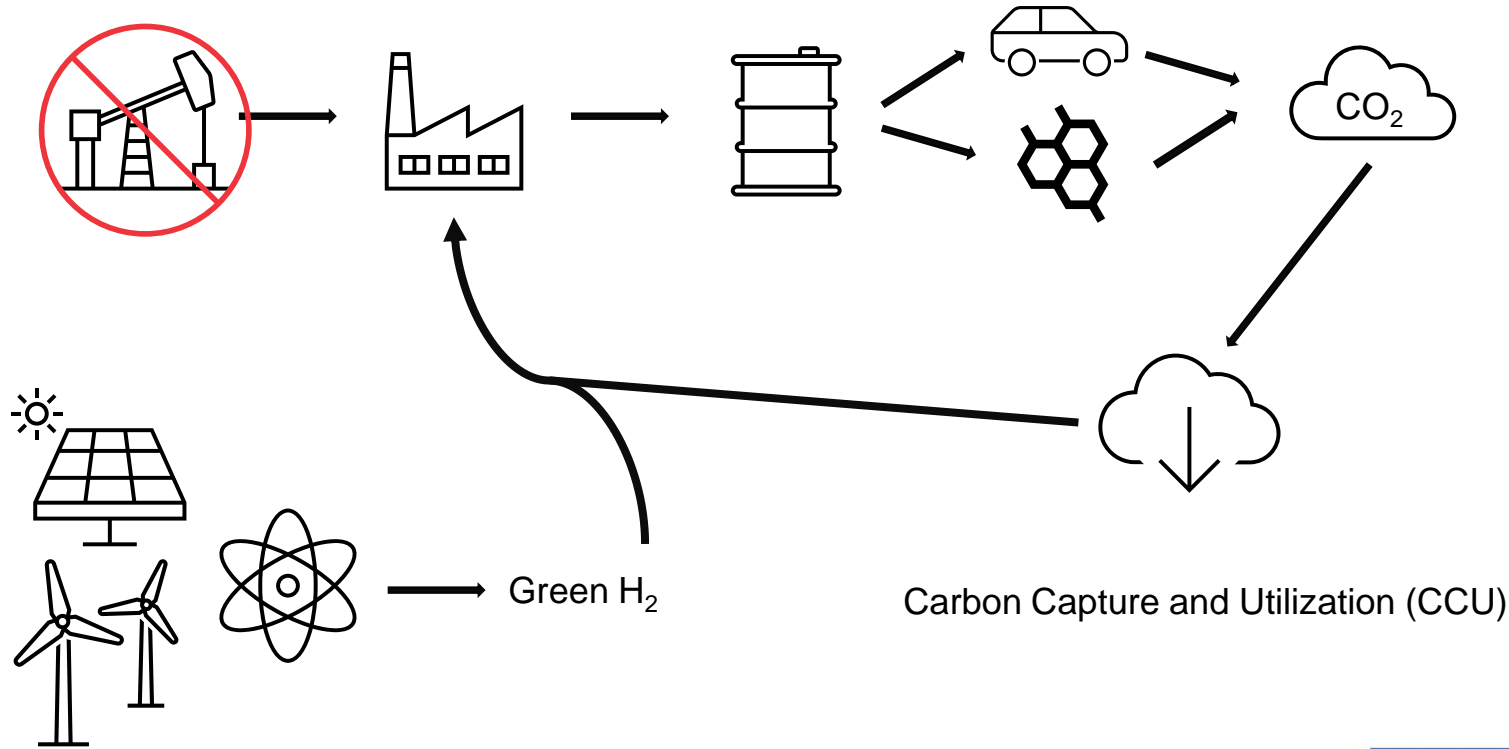
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Aalto-yliopisto
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Aalto University



,chemistry flask with computer code in the background?', Copilot, 28.11.24



Linear and Circular Carbon Economy

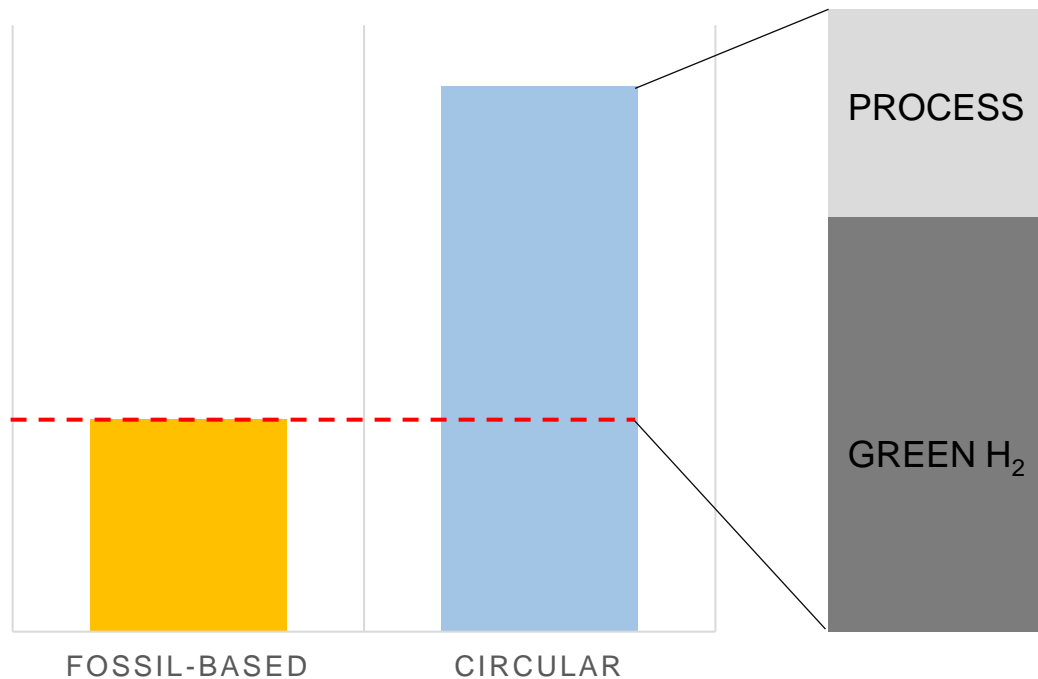


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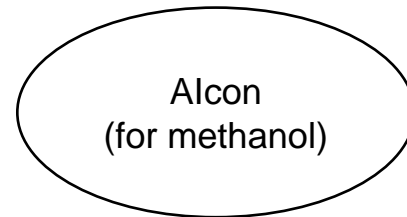


Funded by the
European Union
NextGenerationEU

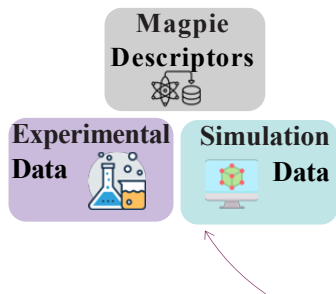
Reducing the cost



- New catalysts
- Improved processes

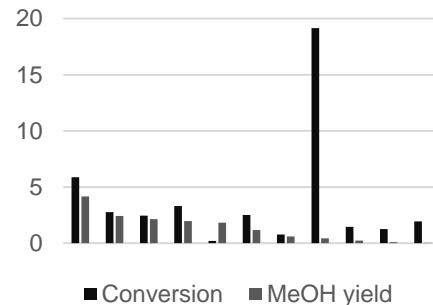
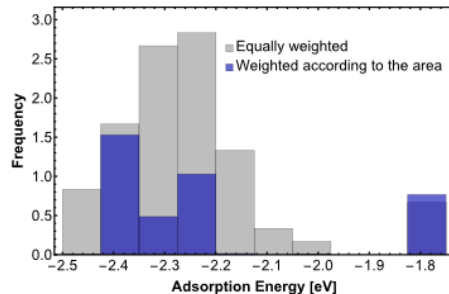


The Alcon Approach



Achievements:

- ✓ Developed simulation and ML workflow
- ✓ Created database
- ✓ 2 catalyst prediction-synthesis-test rounds
- ✓ Process optimized for several catalysts
- ✓ Successful research visit of 2 scientists in the US
- ✓ 8 presentations/posters at conferences
- ✓ 3 manuscripts in preparation



Collaboration!

Experiments & database creation by Prof. Annukka Santasalo-Aarnio's group



DFT and material search ML framework setup by Prof. Patrick Rinke's group



Thank you!