GENERATIVE AND PREDICTIVE MODELS FOR NEW MATERIALS

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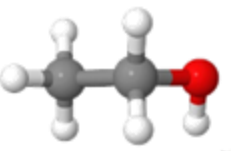
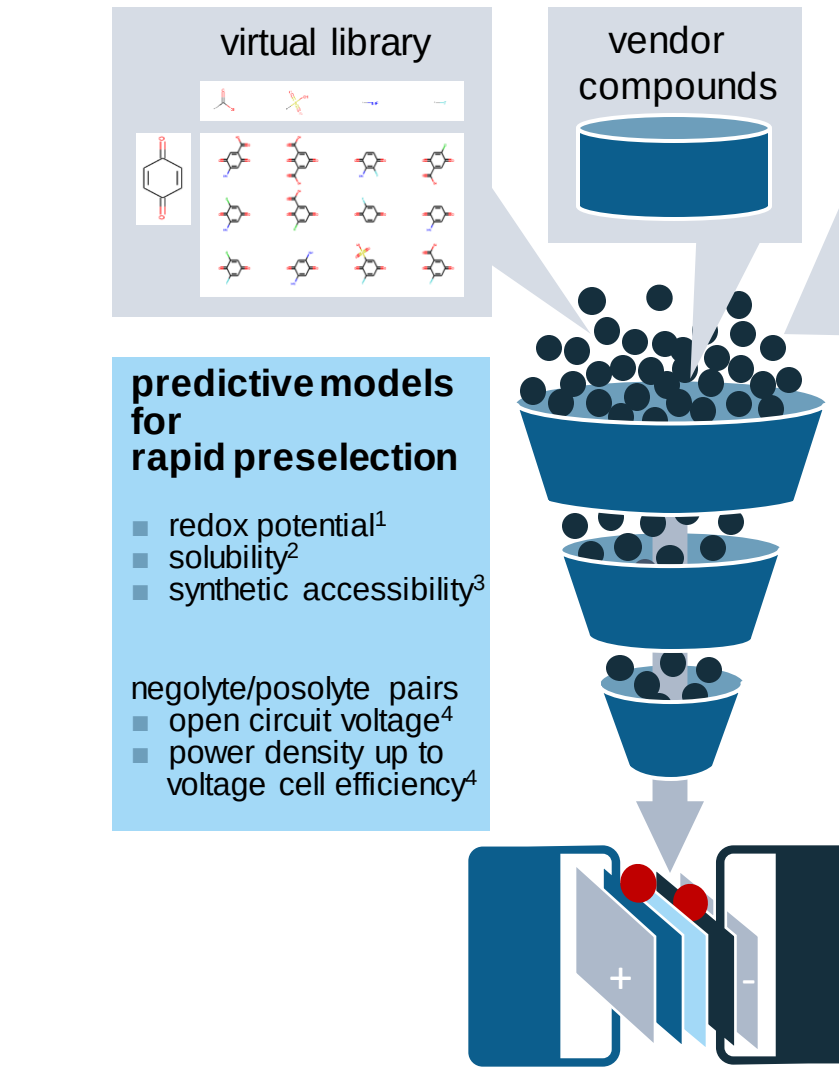
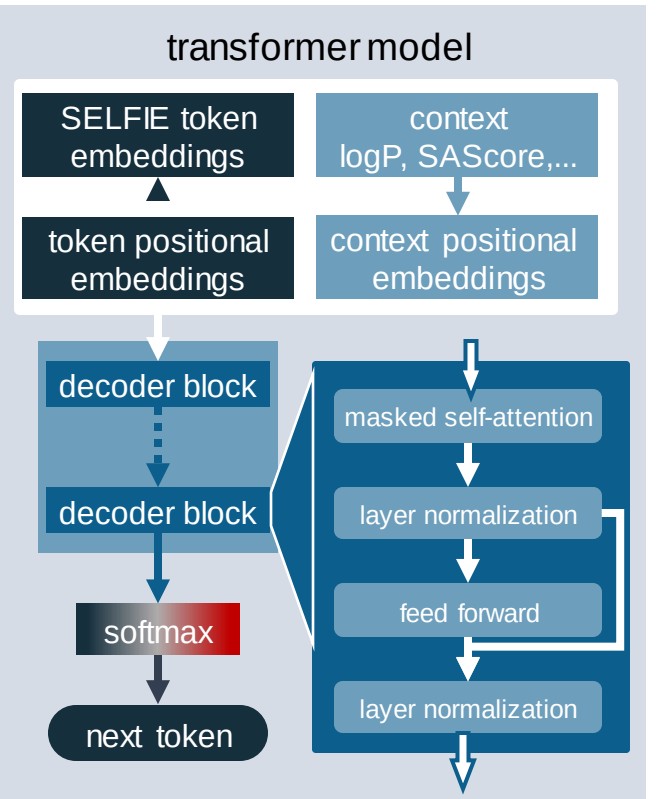


SELFIE: [C][C][O]

C	C	O
C	C	O
C	C	O

masked self attention matrix





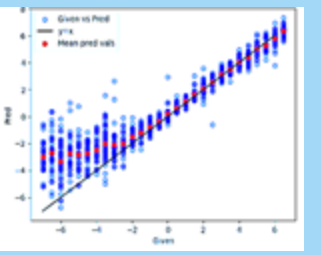
predictive models for rapid preselection

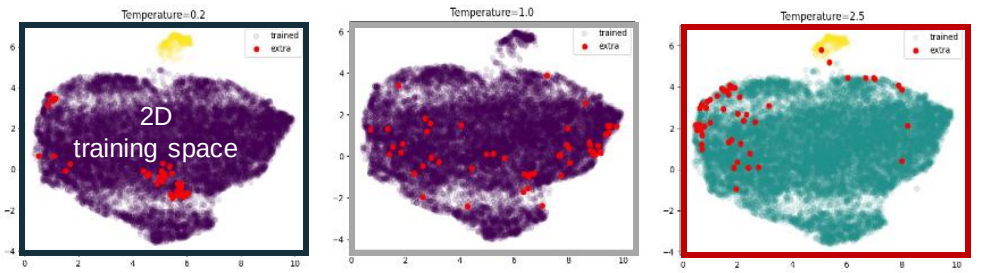
- redox potential[1]
- solubility[2]
- synthetic accessibility[3]

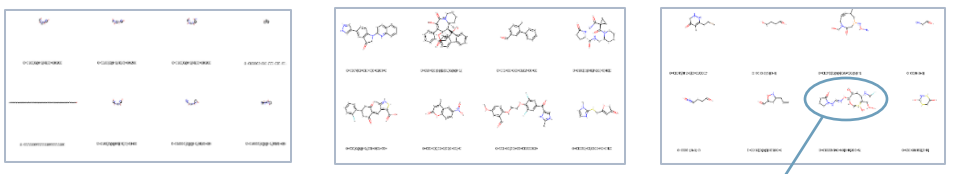
negolyte/posolyte pairs
- open circuit voltage[4]
- power density up to voltage cell efficiency[4]

generative models for new molecules[5,6]

- trained on 13M compounds[7-17]
- + temperature **control variability**
- + context **hit target property**



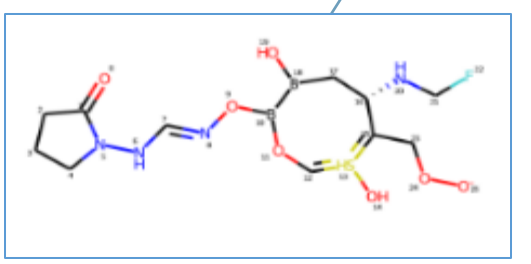




- flexible, python-based workflow, relying on **physical or data-driven models**
- selectable chemistry for redox and/or ageing reactions
- speed up by pre-trained models for PCET reactions
- adaptable sequence of filtering steps
- interface to other modules via JSON
- prototype: **redoxfox.scai.fraunhofer.de**

- outlook: **focus on relevant sub-space by multi-conditional prediction**

quality	%
novelty 10k	98.8
uniqueness 1k	98.7
uniqueness 10k	97.1
validity 10k	100



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This project has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement no. 875489.