Artificial intelligence to discover new chemistries

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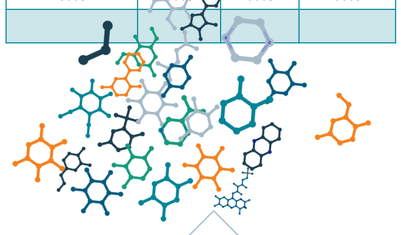
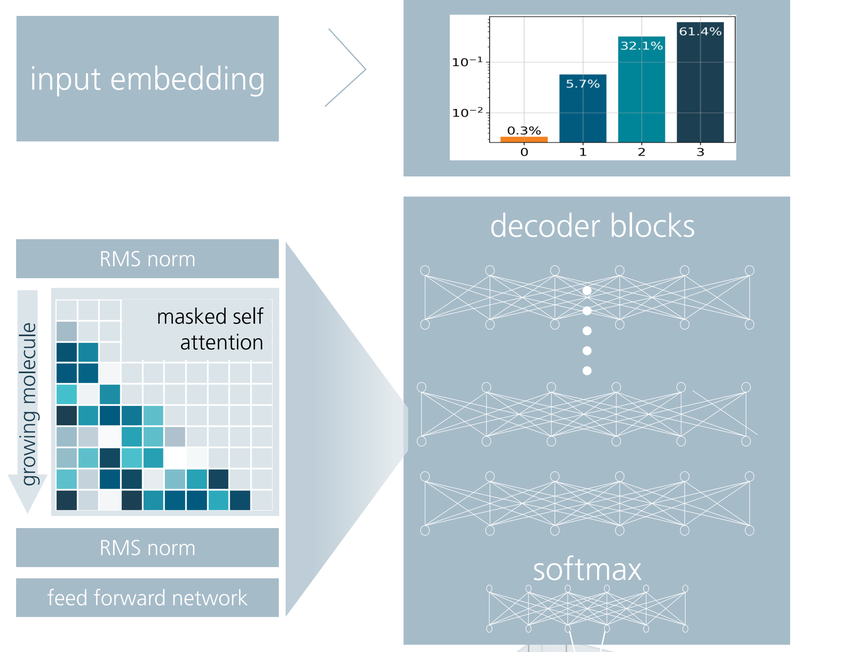
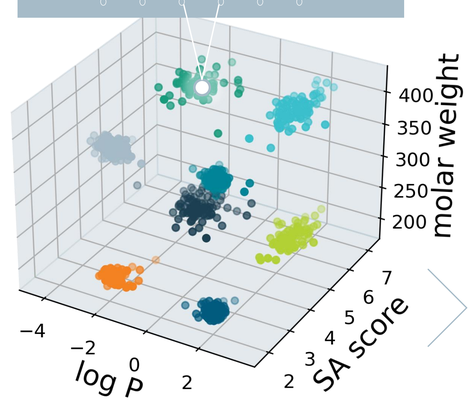
Generative AI for de novo molecular design: LLamol[1]

	Numerical context		
SMILES	logP	SA score	molar weight
C/C=C/CC	1.972	2.88	70
CCC=C(C)C	2.363	2.63	84
….	….	….	….



data set	size
ZINC 15 [3]	5M
QM9 [4,5]	134k
RedDB [6]	31
OPV [7]	91k
PubchemQC [8,9]	5.3M
CEP [10] subset [11]	20k
ChEMBL [12-15]	2.3M
OrganiX13	**12.5 M**





- **generative transformer model** based on LLama2 architecture[2]
  - 8 decoder blocks
  - ~15 M parameters
  - 2 days of training on Nvidia A100 GPU
  - trained on 12.5 M superset of organic compounds
  - new training method **Stochastic Context Learning** for maximum flexibility and robustness
- model handles **single- and multi-conditional** organic molecule generation with up to four conditions
  - valid molecular structures in SMILES notation
  - control creativity via 'temperature' parameter
  - incorporates numerical and/or SMILES sequence
  - easily expandable with new properties

https://github.com/Fraunhofer-SCAI/llamol

condition	novelty %	Uniqueness %	Validity %	MAE
None	89.7	99.9	99.5	-
logP	85.5	99.7	99.4	0.2
SAscore	85.4	98.8	82.1	0.4
molar weight	84.3	99.6	99.4	4

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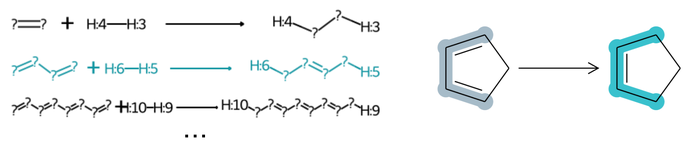
Predictive AI for estimating the redox potential[11]

- chemistry:
  proton coupled electron transfer only: net addition of H_2

$$A_{ox} + H_2 \longrightarrow A_{red} + \Delta E_{DFT}$$

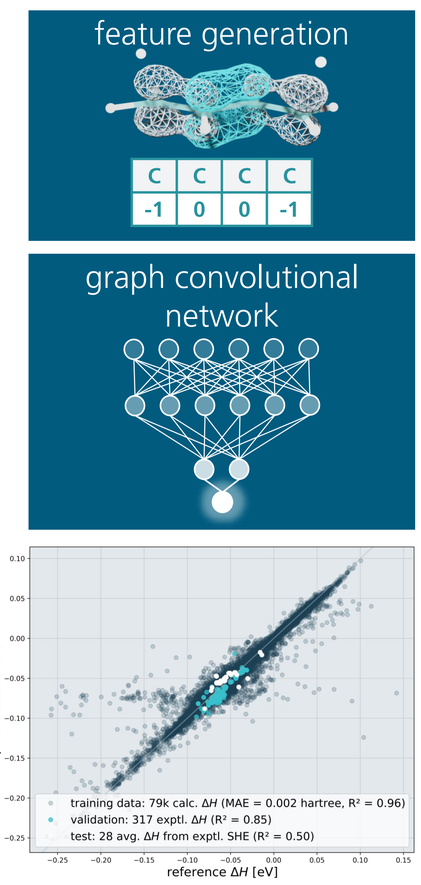
$$E^o = -\frac{\Delta G}{zF} \qquad \Delta G \cong \Delta H_{G4(MP2)} \cong \Delta E_{DFT}$$

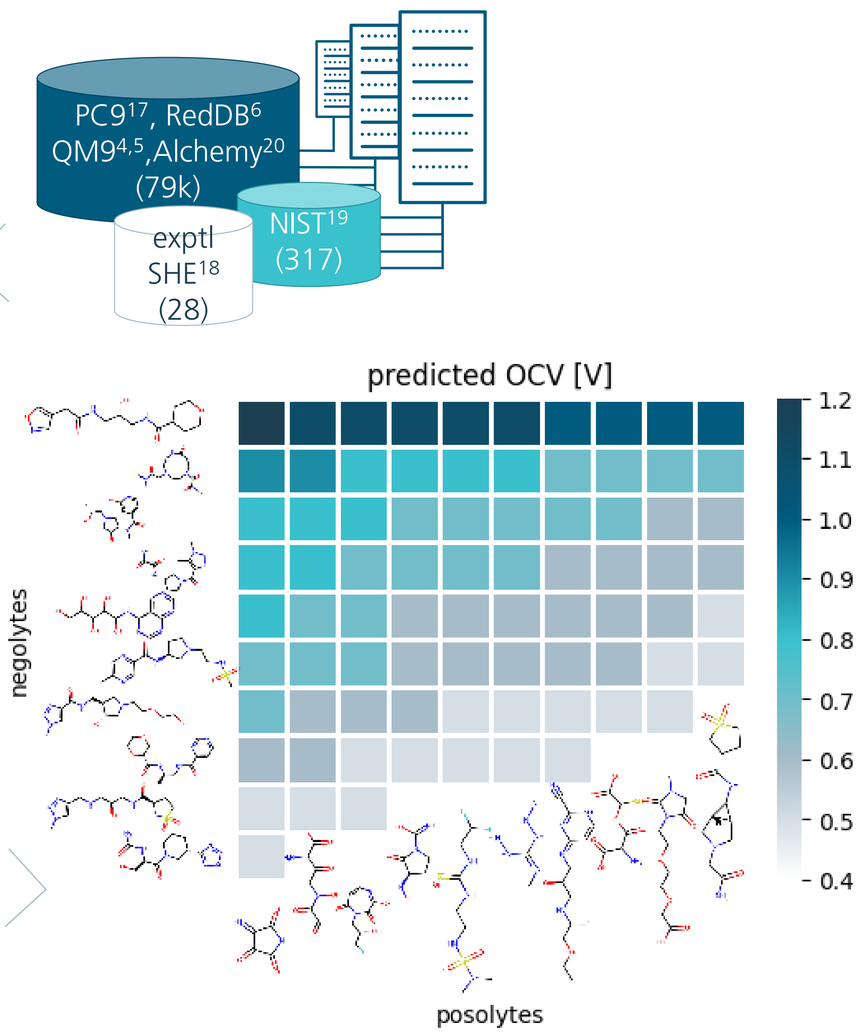
- construct from given molecule A_{ox} reduced form A_{red} via generic reaction templates



- 70 k redox pairs found in precomputed data sets
  - determine
    - **differential features** between A_{ox} and A_{red}
    - **energetic difference** between A_{ox} and A_{red}
- train **graph convolutional network** on molecular features and energy differences
- **predict energy difference** for novel compounds
  - ~50 predictions/sec
  - general trend reproduced[14,15]
  - identify most promising posolyte/negolyte candidates by max OCV

www.redoxfox.scai.fraunhofer.de





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Summary

- prototypic machinery for AI-based creation and evaluatipm of new chemistries in place
- improvements planned
  - generative model: respond to more conditions, train on more relevant properties (e.g. HOMO/LUMO gap)
  - predictive model: train on larger & standardized data; train new model on other properties (e.g. solubility)

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