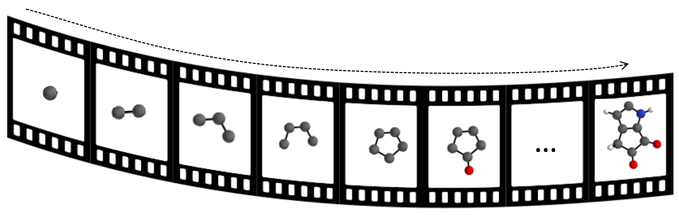
Artificial Intelligence in Theoretical Chemistry
Westermayr Group


Molecular and material design

Goal: use deep generative learning to generate novel structures

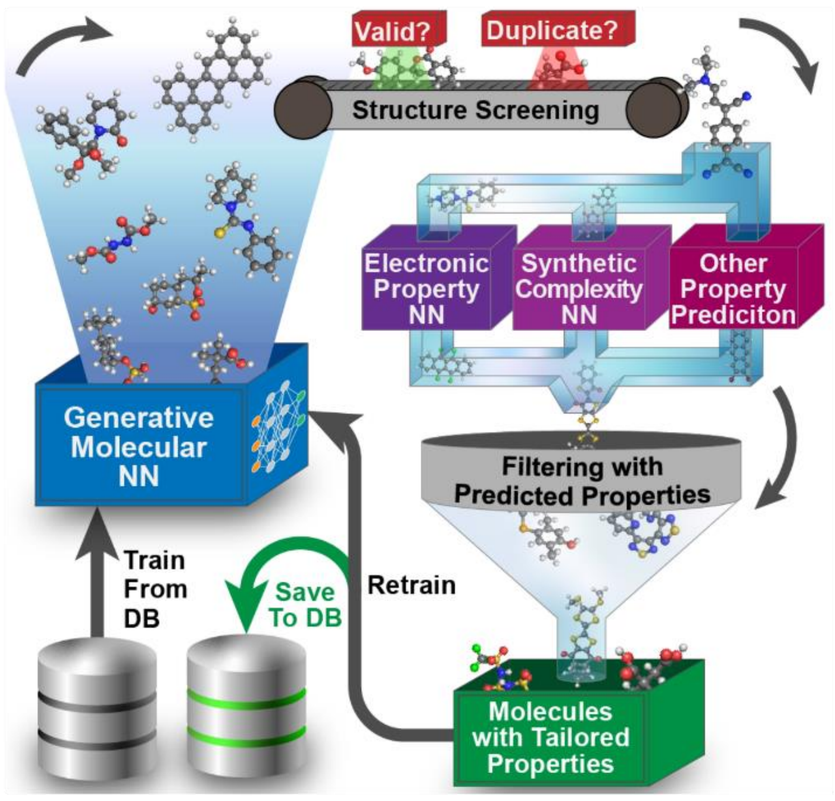
- Conditionally build a molecule atom by atom
- Evaluate new molecules against existing molecules using mathematical descriptors



- We use the cutting-edge molecular generator **G-SchNet**,[1] want to find out more:

Application to molecular material design[2]

We designed new molecules with target properties that are useful for organic electronics.



Generative machine learning models are retrained iteratively to predict molecules with better and better properties.

Future work

- Generation of molecules and materials for CO_2 catalytic conversion
- Design of novel protein structures using AlphaFold.[3]

References:

[1] Niklas W.A. Gebauer, Michael Gastegger, Kristof T. Schütt, "Generating equilibrium molecules with deep neural newtorks", NeurIPS Workshop on Machine Learning for Molecules and Materials 2018.

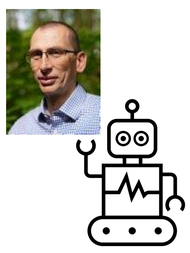
[2] Julia Westermayr, Joe Gilkes, Rhyan Barrett, Reinhard J. Maurer, "High-throughput property-driven generative design of functional organic molecules", arXiv:2207.01476 (2022).

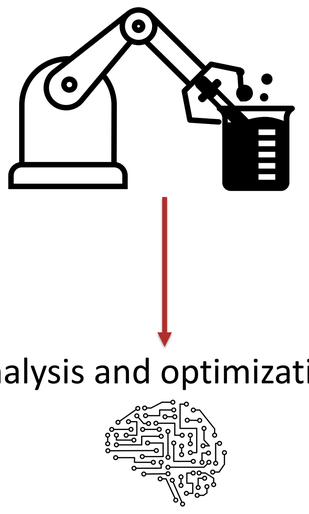
[3] John Jumber et al., "Highly accurate protein structure prediction with AlphaFold", Nature 596, 583 (2021).

AI-driven laboratories

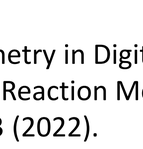
Goal: Using artificial intelligence to drive laboratories and optimize reactions

- In a collaboration with Prof. Belder, we plan to couple artificial intelligence (AI) with a lab-on-a-chip synthesis
- AI should analyse results and optimize reaction conditions





Analysis and optimization



References:

Anish Das, et al. "On-the-Fly Mass Spectrometry in Digital Microfluidics Enabled by a Microspray Hole: Toward Multidimensional Reaction Monitoring in Automated Synthesis Platforms", J. Am .Chem. Sci. 144, 23, 10353 (2022).

Junjie Zhong, et al. "When robotics met fluidics", Lab Chip 20, 709 (2020)

AI-method development: Meta learning

Goal: Improve learning by learning how to learn

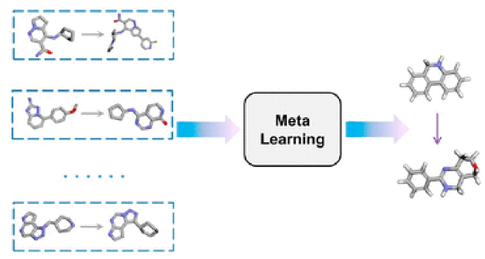
- Is it possible to transfer knowledge between deep learning models studying different molecules and materials?
  - Existing approaches use transfer learning or learn from scratch for every new system

  - What if we want to predict a new molecule? We need to start again.

  - Can we improve and use the knowledge already acquired?

Future work

→ **Meta learning** is learning from a set of tasks in addition to a task itself



- Create meta learning algorithm to predict hyper parameters of model describing different reactions
- Predict weight distribution of new model given previously trained models

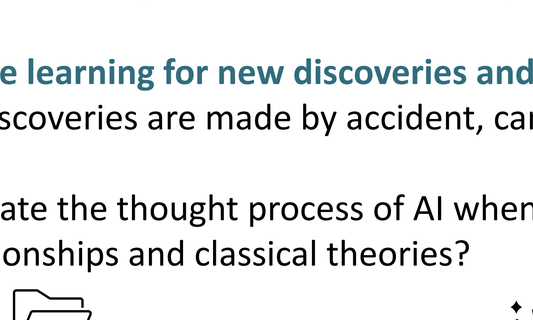
Reference: Thrun, S. & Pratt, L. *Learning to Learn: Introduction and Overview* in *Learning to Learn* (eds Sebastian Thrun & Lorien Pratt) 3-17 (Springer US, 1998).

Reaction discovery

Goal: Using reinforcement learning and other learning methods to discover new reactions and hidden rules in data

Reinforcement learning for reaction discovery

- Learning from interaction with an environment



- Example:
  - A robot learning to play Tetris or chess
  - AlphaGo Zero, which became world leader in the strategy game Go after 40 days of self-playing[1]

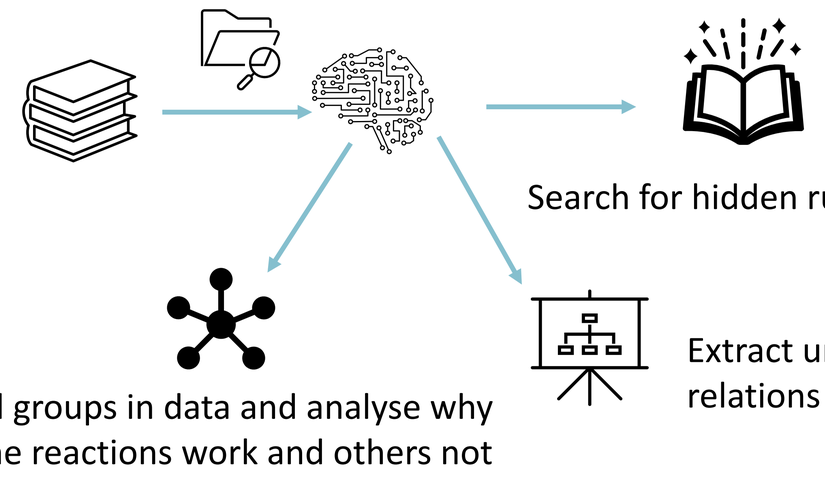
Future work

Reformulate chemical problems as games so AI can learn how to play, some examples include:

- Reaction discovery
- Design of artificial photosynthesis
- Reaction optimization (self-driven laboratories)

Machine learning for new discoveries and data analysis

- Most great discoveries are made by accident, can we use AI to accelerate this process?
- Can we translate the thought process of AI when looking at data into physical relationships and classical theories?



References:

https://www.deepmind.com/research/highlighted-research/alphago

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