Artificial Intelligence Applications in the Design of Novel Dye Molecules with Targeted Optical Properties

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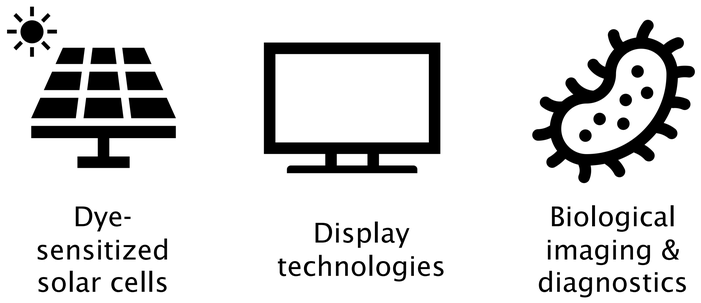
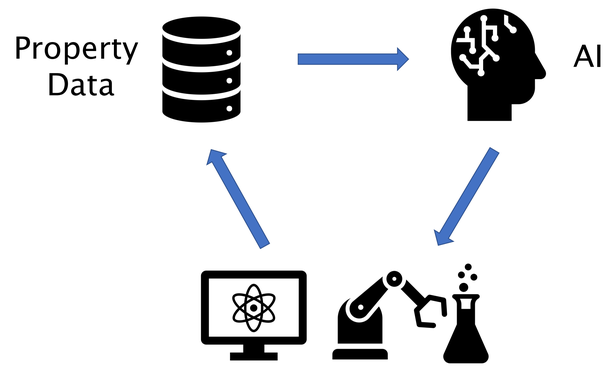
Background

Numerous applications of molecular dyes



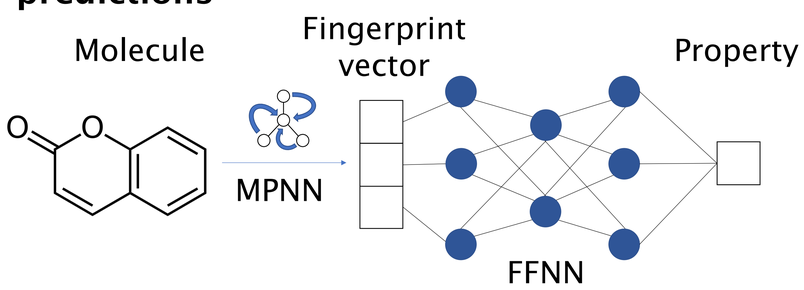
Dye-sensitized solar cells | Display technologies | Biological imaging & diagnostics

AI enables humans to navigate enormous molecular design space



Methods

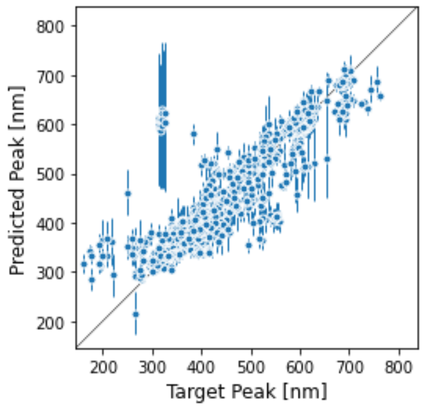
Message-passing neural network (MPNN) learns optimal representation for property predictions[1]



- Molecule represented as a graph (nodes & edges)
- "Messages" passed between neighboring atoms to learn chemical environment
- Aggregate atom vectors to get molecule vector
- Use traditional neural network on property regression problem

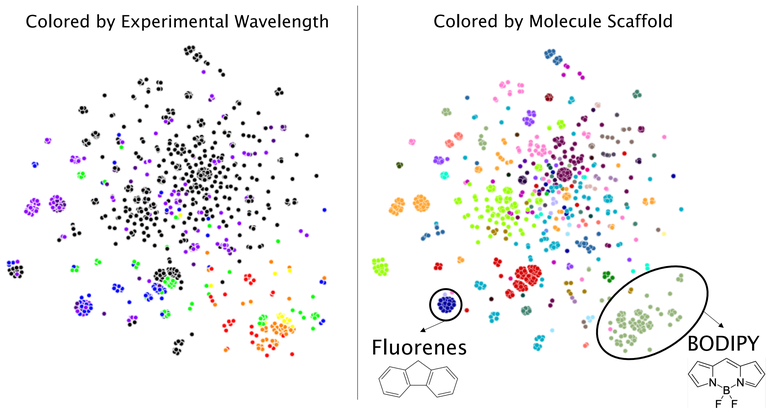
Results

MPNN predicts peak absorption wavelength accurately

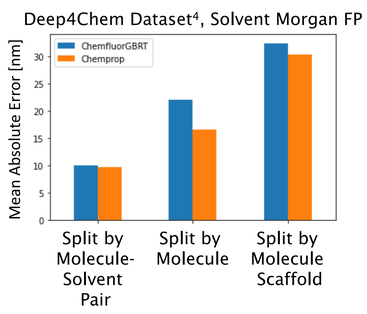


- MPNN outperforms physics-based methods (TD-DFT)
- Uncertainty from ensemble variance provides estimate of model's confidence in each prediction

MPNN embeddings are interpretable in 2-D



Predictions are generalizable to unseen chemistries



- Different train-validation-test split types assess generalizability
- MPNN method is superior to existing statistical methods[3]

Conclusions

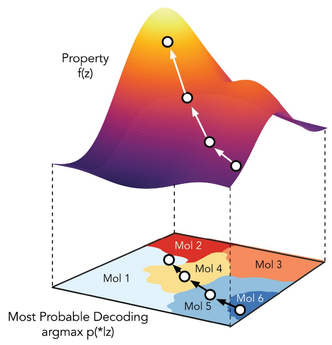
- MPNN method produces accurate, generalizable predictions of the peak absorption wavelength
- This method can be extended to predict other optical properties of interest in molecular dye design

Ongoing & Future Work

Active Learning

- Even with high-throughput techniques, gathering new data is expensive and time-intensive for large libraries
- Active learning uses model uncertainty to determine which new datapoints would be most useful to measure for model improvement

Inverse Design with Generative Models



- Generative models can be trained to propose molecular structures as outputs, given a desired property as an input[2]
- Gradient descent/ascent in continuous latent space that maps to discrete molecule space

Autonomous, Closed-Loop System

- Given a molecular design objective, a computer and a robotic experimentalist will make autonomous decisions to pursue that goal

References

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4. Joung, J. F.; Han, M.; et al. *Sci. Data* 2020, *7* (1), 1–6.

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