Accelerating the design and optimization of OLED materials using active learning

OLEDs (Organic Light-Emitting Diodes) are extensively used in digital displays such as those in smart phones, television screens, computer monitors, and game consoles. They contain organic molecules with unique electronic structures that create light in the visible part of the spectrum through a process called electroluminescence. For an OLED to be commercially valuable, it should satisfy several constraints, including high efficiency, low-cost fabrication, and good electrochemical stability for long-term operation, making discovery of novel OLED materials a challenging problem.

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Challenges

Molecular modeling and simulation tools have proven effective in materials discovery and are increasingly deployed in industrial R&D. Although digital simulations have offered tremendous time savings for R&D workflows compared to traditional experimental approaches, several challenges persist:

- The potential chemical space for materials design and discovery is massive, even for highly constrained problems

- Predictions based on density functional theory (DFT) calculations can be laborious and computationally expensive, limiting the number of candidates evaluated within fixed timescales and resources

- It is challenging to maintain a high level of accuracy to properly assess the complexity of materials

Solution: Active Learning Workflows

A new approach is required to guide scientists to the best performing or useful candidates. Thanks to the application of a machine learning (ML) paradigm called "active learning" (AL), Schrödinger has made this problem readily tractable. Recently, Schrödinger has developed active learning workflows which leverage the synergy between physics-based simulations and machine learning for optoelectronic properties predictions. The active learning workflow enables scientists to zoom in on the "best-performing" portion of a given sample space in a more efficient and cost-effective manner. The workflow allows:

- Automated active learning calculations with minimum users input

- Accounting for multiple optoelectronic parameters simultaneously for materials discovery

- Combining active learning with DFT to efficiently identify materials with optimal properties

- Employing built-in descriptors and fingerprints to featurize chemical structures

- Building high-performance ML models using adaptive design procedures

- Minimizing the number of time-consuming physics-based calculations

"The AL workflow enables accelerated design and discovery of optoelectronic materials. The workflow is fully automated, significantly reducing the number of physics-based simulations to predict materials properties in an extensive library. The rapid screening of datasets allows a better understanding of structure-function relationships for systematic design and application of optoelectronic materials with higher efficiency."

—Hadi Abroshan, Senior Scientist, Schrödinger

Case Study

Recent studies by Schrödinger, published in Frontiers in Chemistry and presented at SID-Display Week 2022, have demonstrated the active learning paradigm for OLED materials discovery.[1,2]

To explore the best performing hole-transporting molecules for OLED, scientists screened a large pool of 9,000 molecules using the automated active learning workflow. The initial training set included 50 molecules for which a machine learning model was developed supporting efficient multi-parameter optimization (MPO). The ML model was then used to predict the rest of 8,950 molecules in the pool, each of which only costs a fraction of second. Top 50 molecules with higher MPO score and uncertainty were selected for DFT calculations and the calculated data were input for the next iteration of ML model training. The size of the training set for active learning was increased from 50 to 550 molecules in 10 iterations.

Active learning is the iteration of these steps until the DFT calculated data and the machine learning predicted data converge with sufficient accuracy. By using the AL approach, the scientific team was able to screen the chemical space of the materials library 18 times faster than the traditional approach of expensive quantum mechanical calculations, leading to considerable time and resource savings.

The Active Learning Workflow

Validated top-ranked ML predictions

Top 50 molecules with higher MPO score and uncertainty were selected for DFT calculations

Make predictions and calculate uncertainties of remaining molecules

Develop ML models support MPO

Data for ML Models

The Active Learning Loop

10 iterations 50–550 molecules

Randomly select 50 structures

9000 Materials Structures
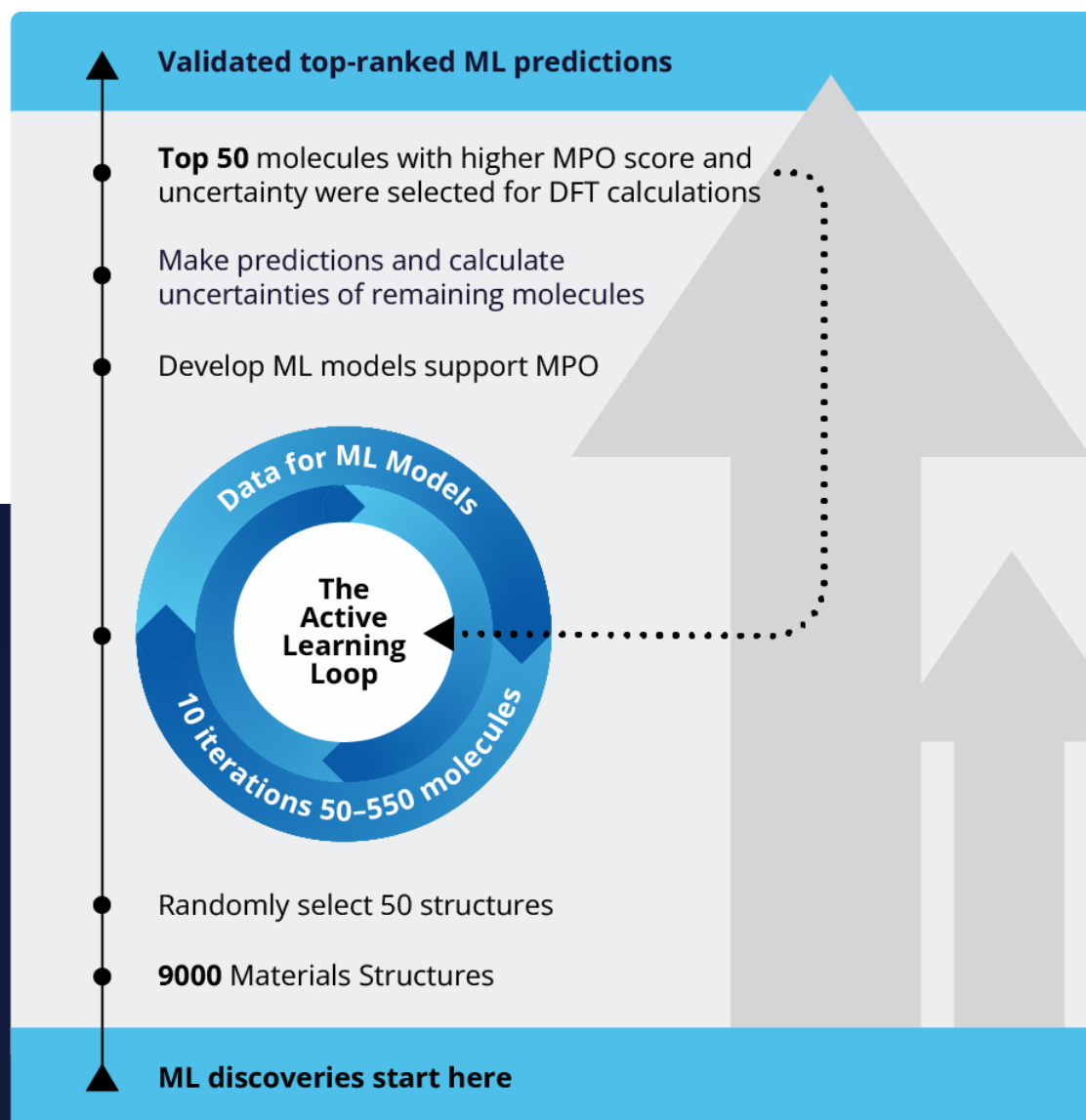
ML discoveries start here

Diagram of the automated active learning workflow for the design and discovery of novel OLED materials

References

1. Active Learning Accelerates Design and Optimization of Hole-Transporting Materials for Organic Electronics
Hadi Abroshan, H. Shaun Kwak, Yuling An, Christopher Brown, Anand Chandrasekaran, Paul Winget and Mathew D. Halls, *Front. Chem.,* 2022, 9, 800371

2. Active Learning for the Design of Novel OLED Materials
Hadi Abroshan, Anand Chandrasekaran, Paul Winget, Yuling An, Shaun Kwak, Christopher T. Brown, Tsuguo Morisato, and Mathew D. Halls, *SID Symposium Digest of Technical Papers,* 2022, 53, 885-888

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