Friedrich-Alexander-Universität Erlangen-Nürnberg

Predicting untrained material combinations by linking spectral features to efficiency parameters using gaussian process regression (GPR)

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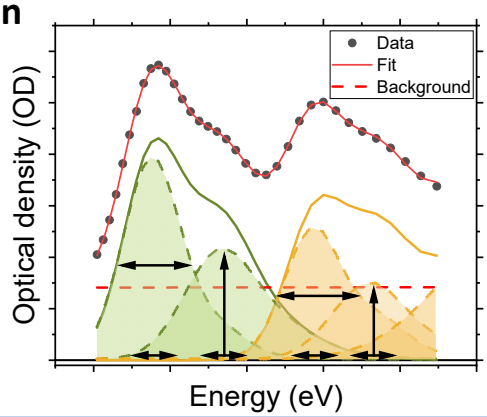
Motivation

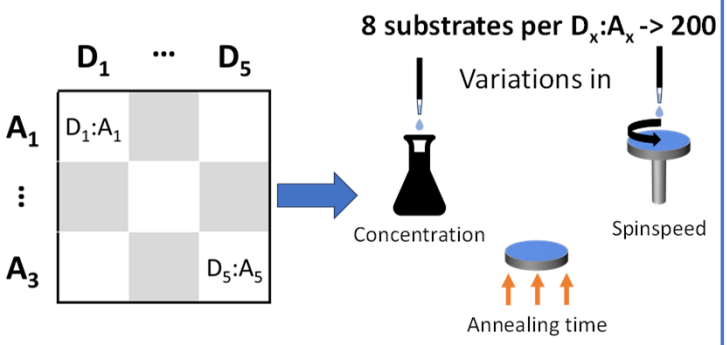
- OPV has vast possibilities of active layer combinations
- Testing all combinations would require unfeasible amount of time
- Structure-property relationship was successfully used in other material sciences to speed up research progress
- UVVIS can provide the structure component by being non-destructive, easy and fast

Spectral deconvolution

- A UVVIS spectrum of an active layer material consist of multiple spectral bands
- Bands are caused by differently aggregated phases in the acceptor and donor
- These aggregates are normal distributed and can be deconvoluted by gaussian peaks
- Smart selection of free parameters for the gaussian peaks necessary to prevent crosstalk

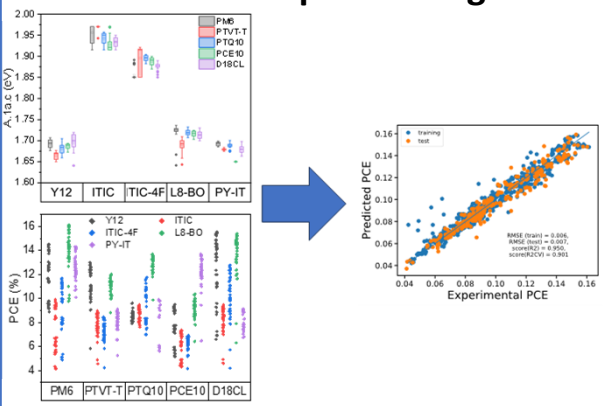


Experiment design



- 5 Donors and acceptors -> 25 combinations
- 8 different substrates per combination

Gaussian process regression

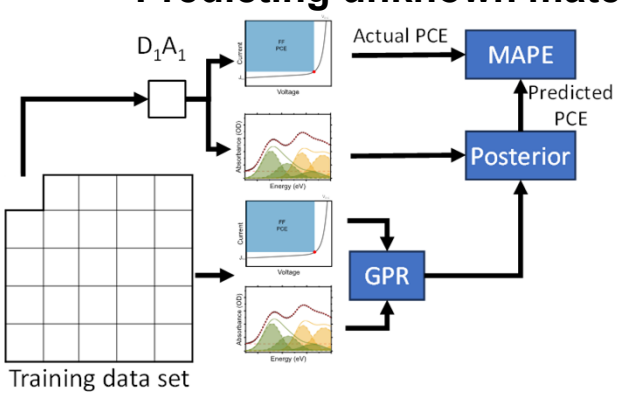


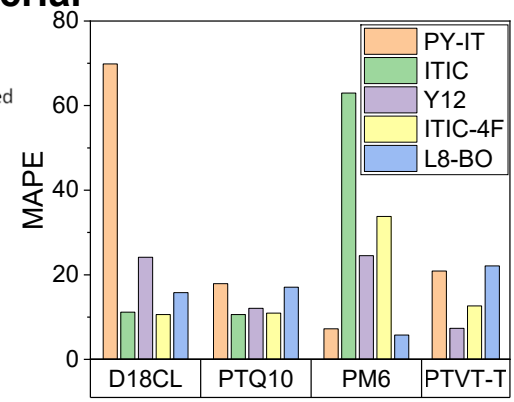
- All spectral data and IV values used to train the model -> R^2 of 0.95, RSME < 0.01

Predicting unknown material

1. Comparison of real vs predicted IV
2. Excluding one combination
3. Training the rest of the dataset
4. UVVIS used to predict IV

-> Mean absolute error (MAPE) partially under 20%





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