

Machine Learning Enables Prediction of Polymer Miscibility by Modeling Polarity Scales

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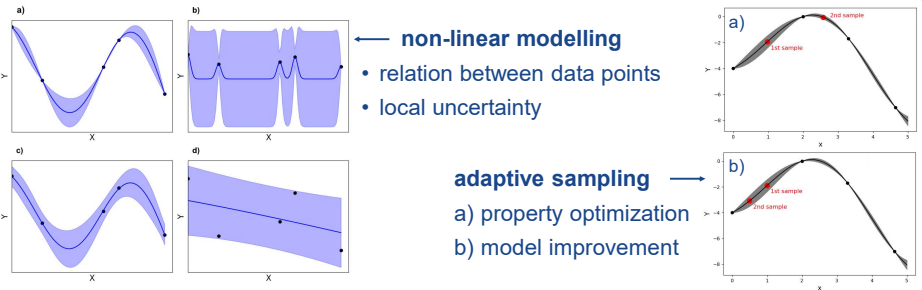
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Introduction

- Polarity influences solvation and phase separation in mixtures
- Hansen solubility and solvatochromic methods consider interaction forces for polarity determination
- Machine Learning offers flexible modelling predicting polarity in multi-component systems

Machine Learning - Gaussian Processes



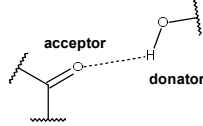
Background – Polarity Parameters



Solvatochromic dyes

- absorption/colour depends on the polarity of surrounding medium
- UV/Vis in solvents
- UV/Vis in polymer/resin films

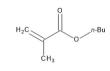
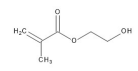
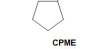
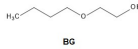
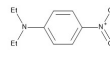
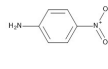
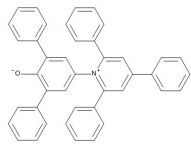
α - hydrogen bond acceptor
 β - hydrogen bond donor
 π^* - dipolarity/polarizability



Materials

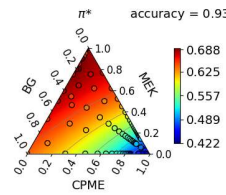
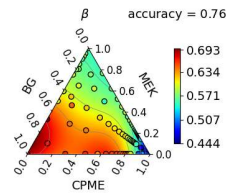
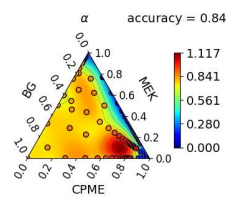
- dyes / probes
- solvents
- copolymers

- α, β, π^* for
- solvent mixtures
 - ternary copolymers

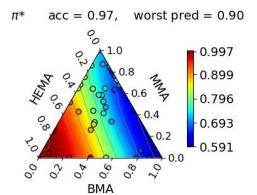
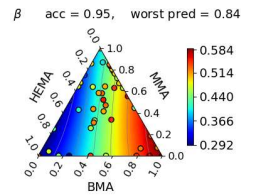
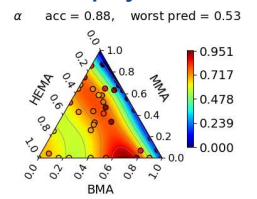


Modelling of Ternary Systems

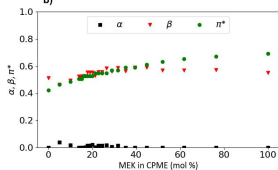
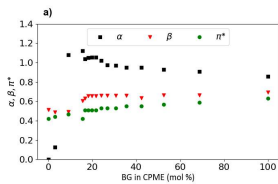
Solvent mixtures



Copolymers

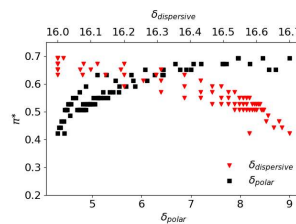
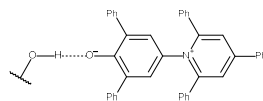


Kamlet-Taft parameters of solvent mixtures & relation to HSP

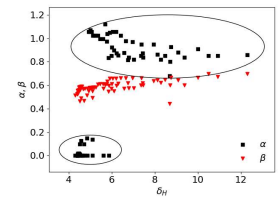


Binary mixtures

- β, π^* describe polarity with sufficient precision
- α strongly effected by hydrogen bonding to the OH-group of BG
- preferential solvation of **Betaine 30** in H-bond donating matrices



$\pi^* = \bar{\delta}_{\text{polar}} \mid \pi^* = \bar{\delta}_{\text{dispersive}}$
Kamlet-Taft: one parameter for dipolarity/polarizability



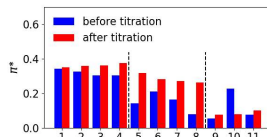
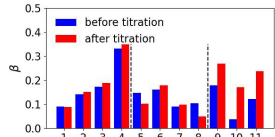
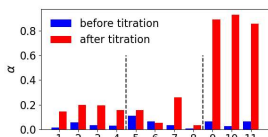
$\alpha - \delta_H \mid \beta - \delta_H$
Kamlet-Taft: differentiate between H-bond acceptor/donor

Turbidity Titration

- titration of polymer solution
- prediction polarity parameters of final solvent mixture

1-4: high HEMA titrated against CPME
5-8: medium HEMA titrated against CPME
9-11: no HEMA titrated against BG

- polarity shift must be considered individually for each case
- 1-4 and 5-8: shift of π^* important, but different threshold values
- 9-11: shift of α and β significant, challenged by preferential solvation



Conclusion

- active learning delivers accurate predictions with smallest possible experimental scope
- Kamlet-Taft provides insights into interactions between molecules
- together with HSP broadens the application in solvation studies
- **Outlook:** Macroscopic property modeling underway using formulation and polarity parameters as inputs