Organic Solvent Nanofiltration and data-driven approaches

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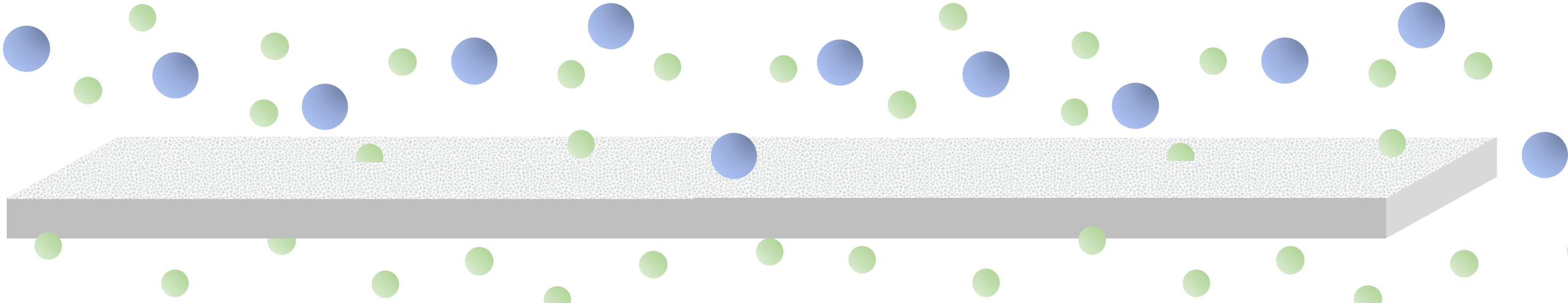
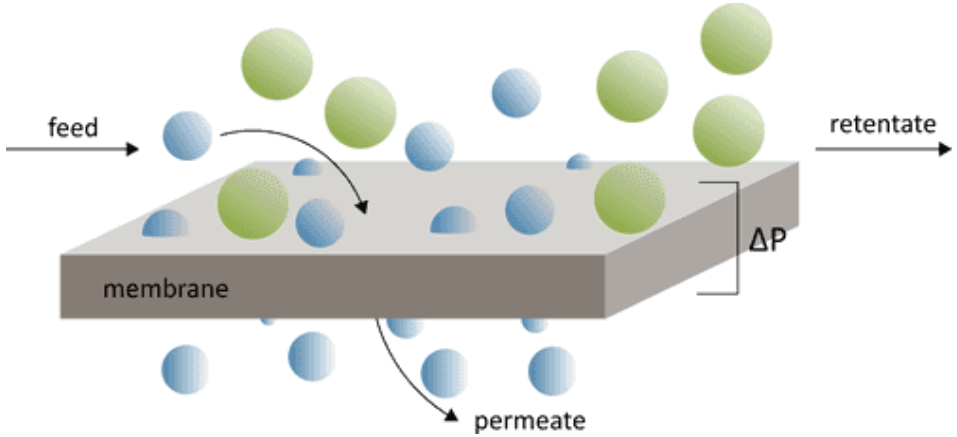


Membranes are strong and sustainable separation tools

An alternative to ubiquitous distillations and evaporations:

- Energy and CO_2 reduction
- Easy scalability
- Hybrid processing possible

Distillation Tower



Membrane separation

Origins in water separation

For example: Desalination,
getting salt out of seawater

- Reverse Osmosis: Membrane separation
- Model-based understanding
- E.g., Spiegler-Kedem model

Membranes for desalination

Origins in water separation

For example: Desalination,
getting salt out of seawater

- Reverse Osmosis: Membrane separation
- Model-based understanding
- E.g., Spiegler-Kedem model:

Linear irreversible thermodynamics:

$$J_w = L_{11}F_w + L_{11}F_s$$
$$J_s = L_{21}F_w + L_{22}F_s$$

Origins in water separation

Linear irreversible thermodynamics:

$$J = L(\Delta p - \sigma \Delta \pi)$$

$$J_s = -P\Delta z \frac{dc}{dz} + J(1-\sigma)c$$

$\longleftarrow$

$$J_w = L_{11}F_w + L_{11}F_s$$

$$J_s = L_{21}F_w + L_{22}F_s$$

With *volume* flux $J = \nu_w J_w + \nu_s J_s$

Origins in water separation

FLUX:

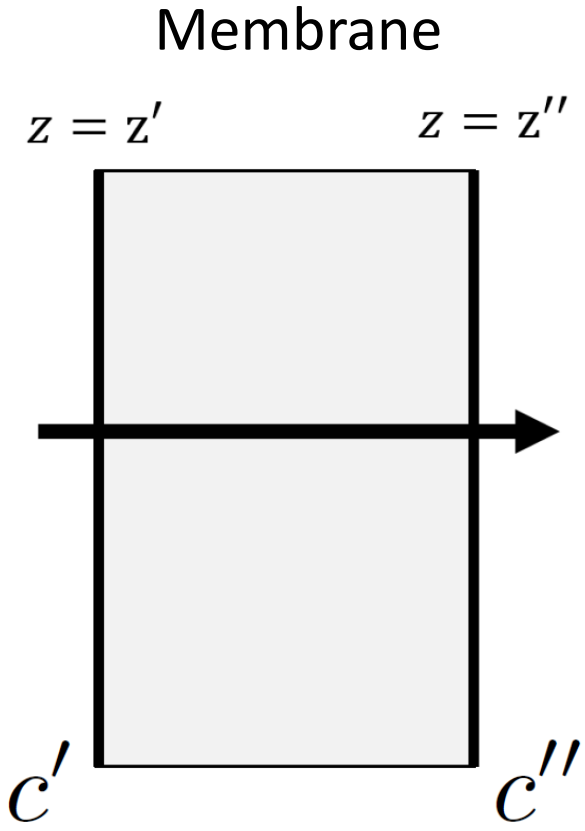
$$J = L(\Delta p - \sigma \Delta \pi)$$

$$J_s = -P\Delta z \frac{dc}{dz} + J(1-\sigma)c$$

RETENTION:

$$R = 1 - \frac{c''}{c'}$$

With *volume* flux $J = \nu_w J_w + \nu_s J_s$



Origins in water separation

FLUX:

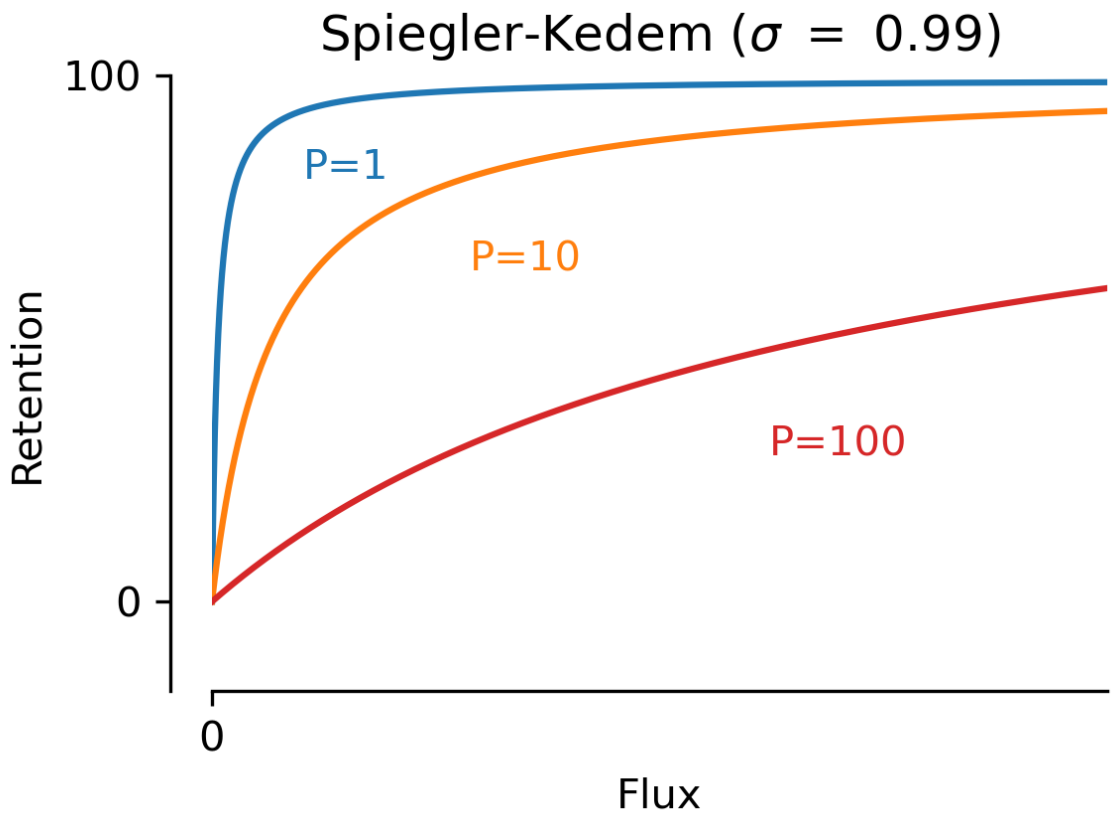
$$J = L(\Delta p - \sigma \Delta \pi)$$

$$J_s = -P\Delta z \frac{dc}{dz} + J(1-\sigma)c$$

RETENTION:

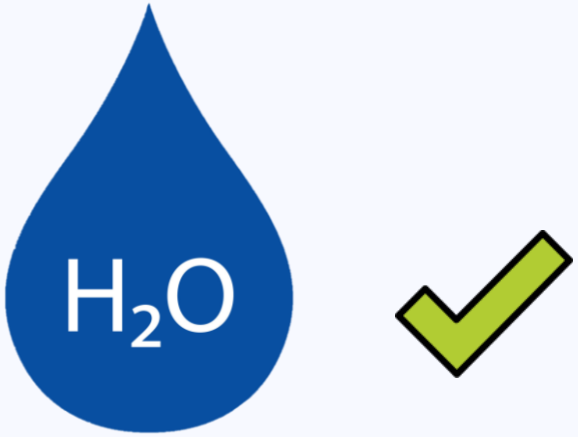
$$R = \left[\frac{1 - e^{-\frac{J(1-\sigma)}{P}}}{1 - \sigma\, e^{-\frac{J(1-\sigma)}{P}}} \right] \sigma$$

With *volume* flux $J = \nu_w J_w + \nu_s J_s$

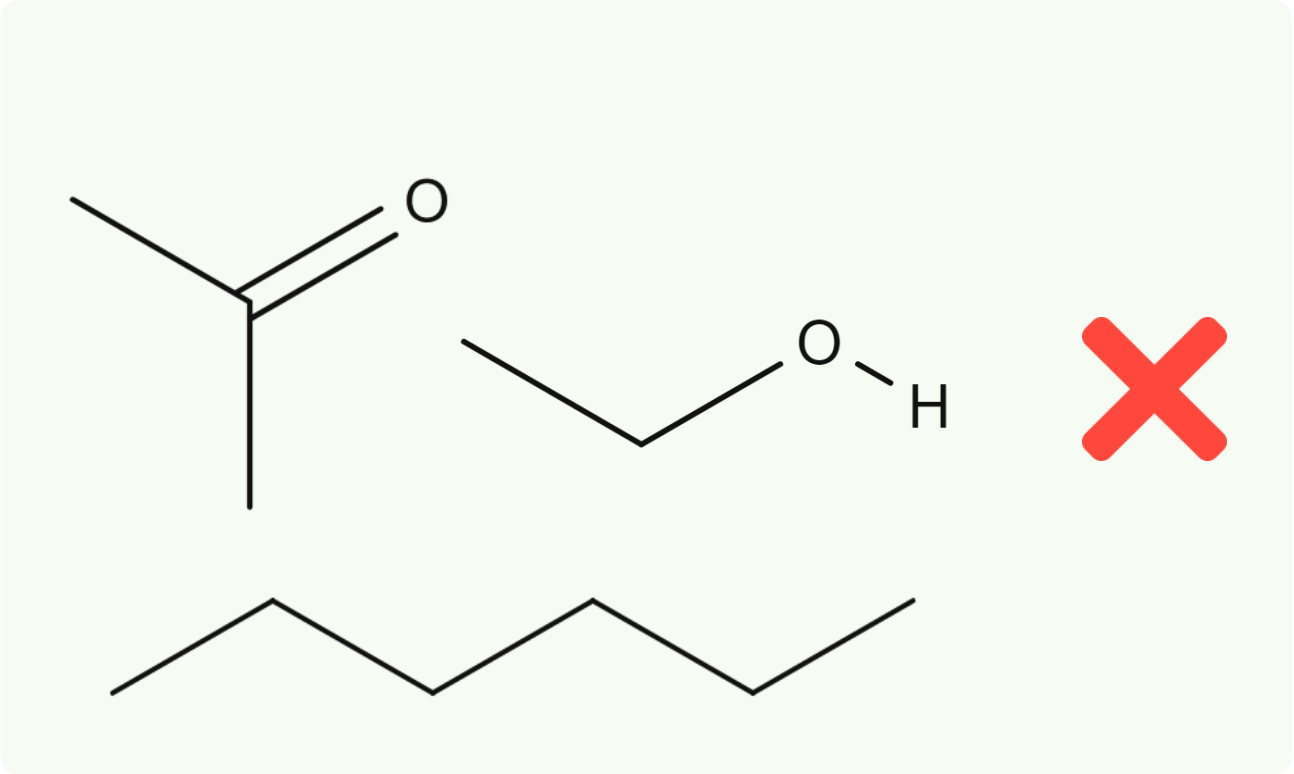


Model is *not* predictive for just any solvent

Works well for **water**



Loses predictive ability
for **organic solvents**



Model is *not* predictive for just any solvent

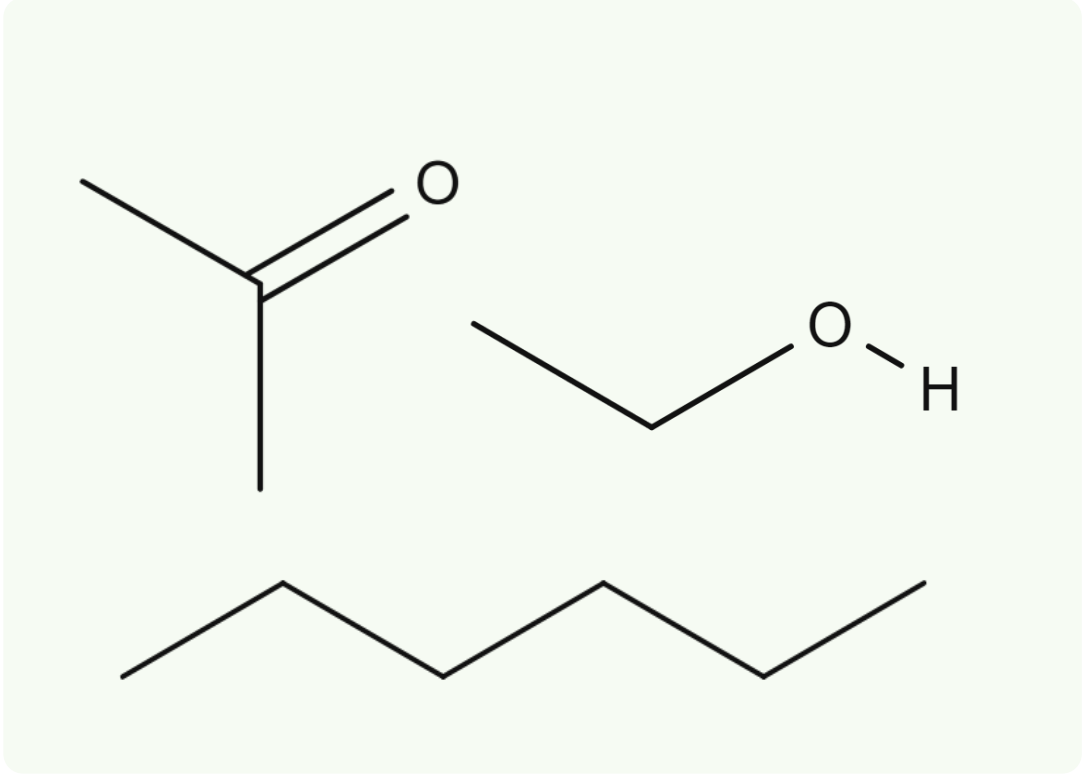
Complex separation mechanism

Interactions between solvent-solute-membrane

Nanoscale: ‘pore’-size reached molecular level

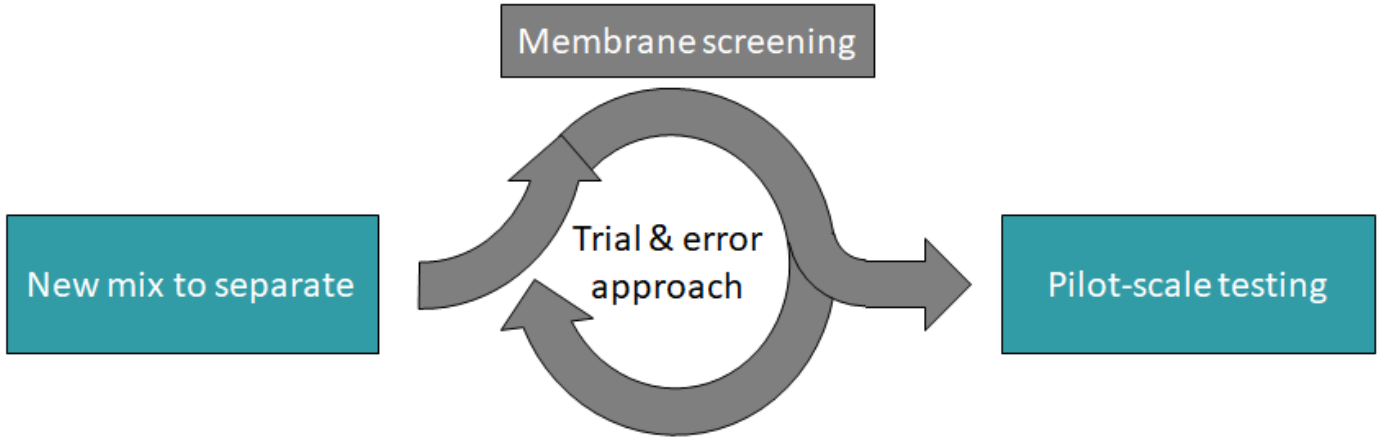
→ Model is not able to generalize for just any solvent

Loses predictive ability for **organic solvents**



Slow development process hampers industrial acceptance

Despite advantages of sustainability of membranes, there is a catch…



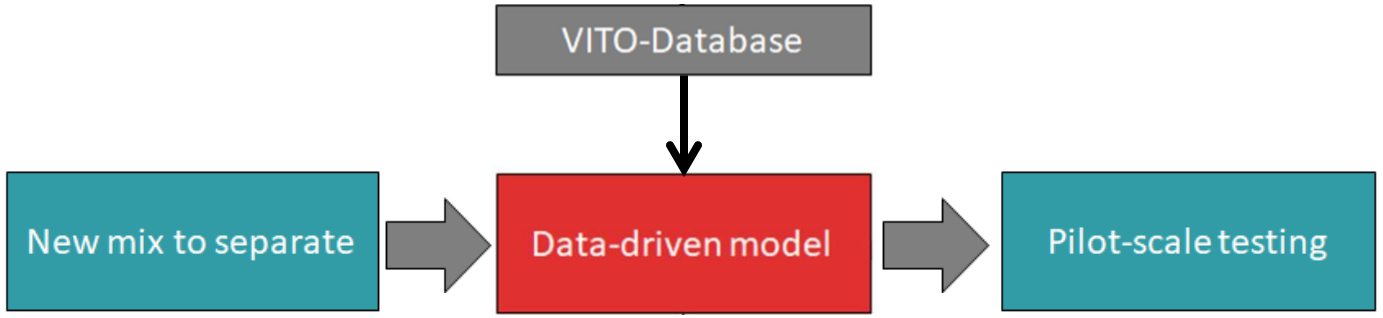
Data driven approaches to the rescue

Unique database

Data-driven models
for prediction

Physical understanding

→ Speed up the
development process



Ceramic Membranes: our Advantage

Unique compared to common polymeric membranes:

- Inert
- No swelling
- Simpler separation mechanism

Data driven approaches for understanding and prediction

- Exploratory data-analysis
- Dimensionality reduction
- **Predicting membrane performance**

Descriptors

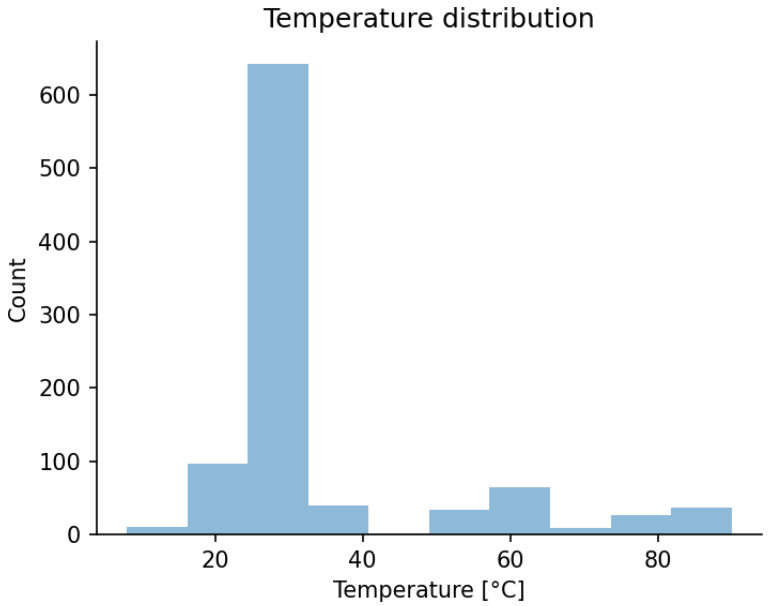
SOLVENT	MEMBRANE
Category	Contact angle
Density	Functionalization
Hansen Solubility Parameters	Hansen Solubility Parameters
Kinetic Diameter	Material
Molar Volume	MW cut-off
Molecular Weight	Polarity
Viscosity	Pore size
	Water permeability
SOLUTE	**TEST CONDITIONS**
Hansen Solubility Parameters	Concentration of solute
Isomeric Smiles	Crossflow
Molecular Weight	Pressure (TMP)
Polarity	Temperature
Structure	

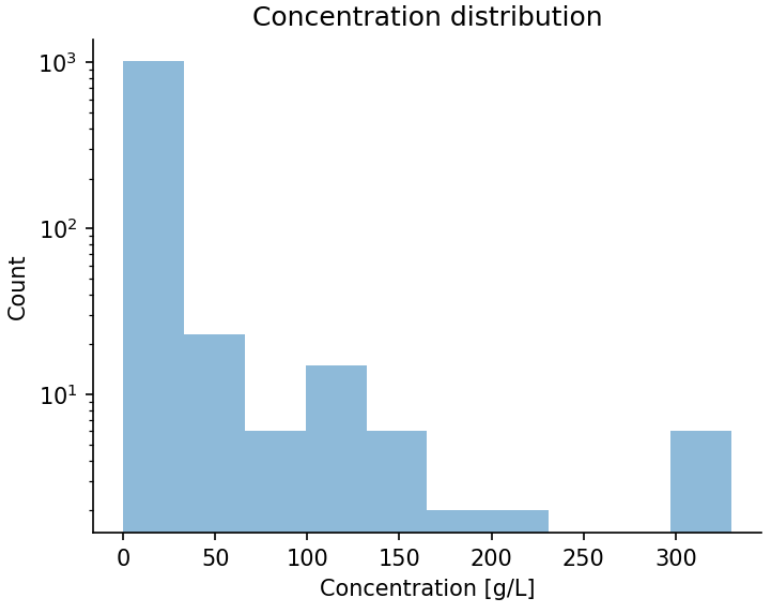
Descriptors

Data-driven model

Retention
Flux

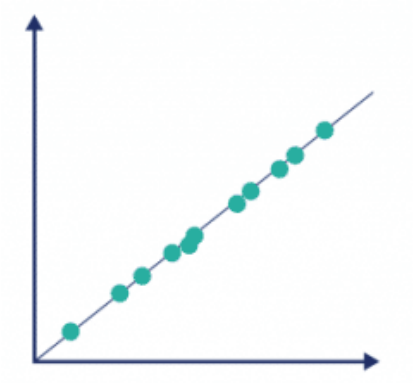
The data distribution dictate the limits of our model



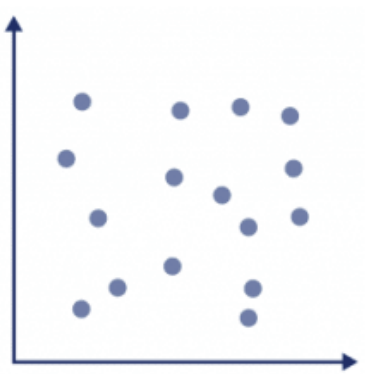


Correlations among descriptors

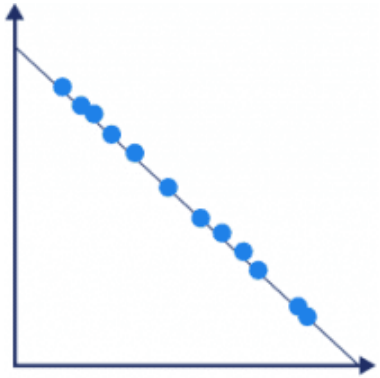
Strong Positive Correlation



No Correlation



Strong Negative Correlation

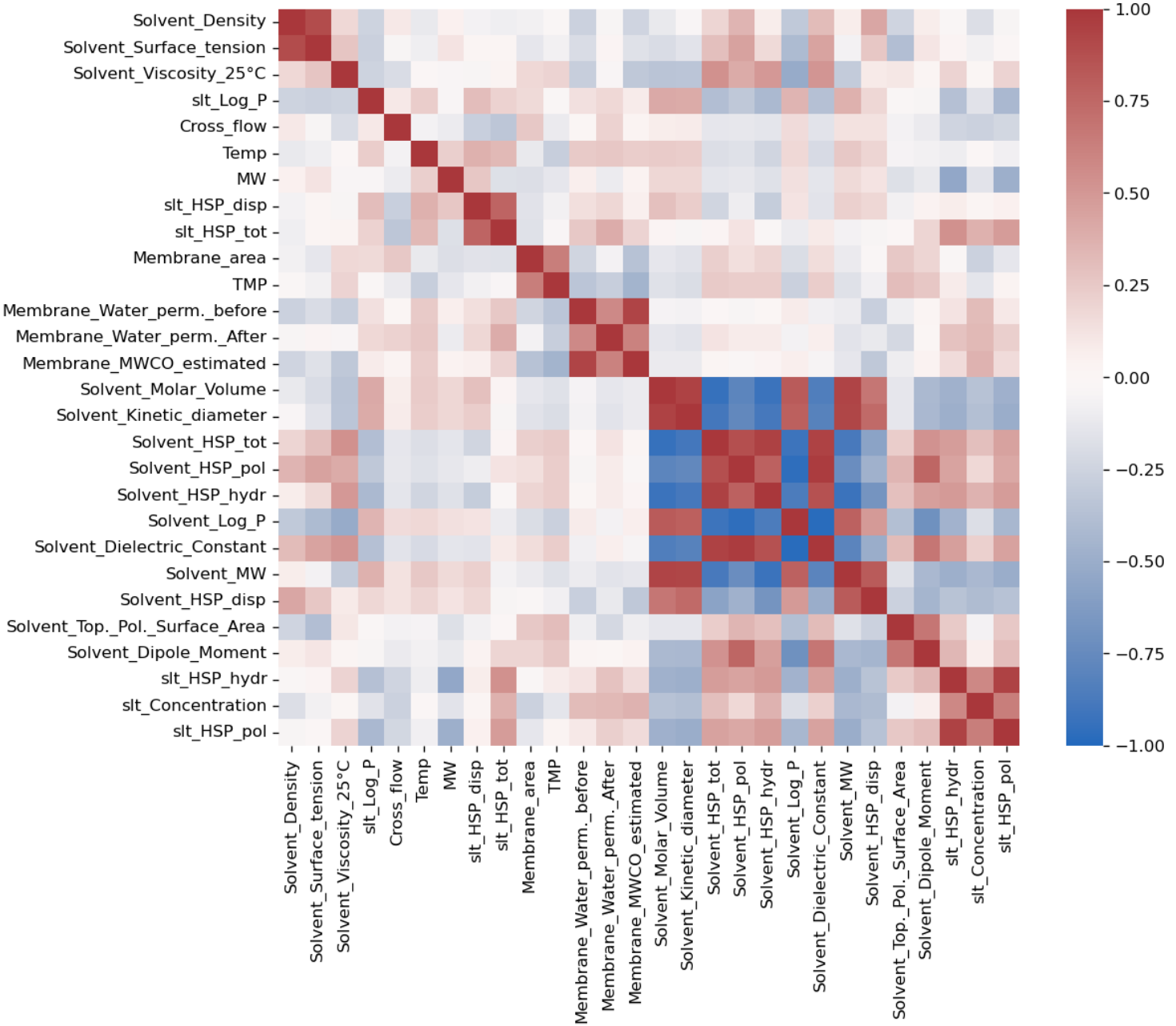


+1 **0** **-1**

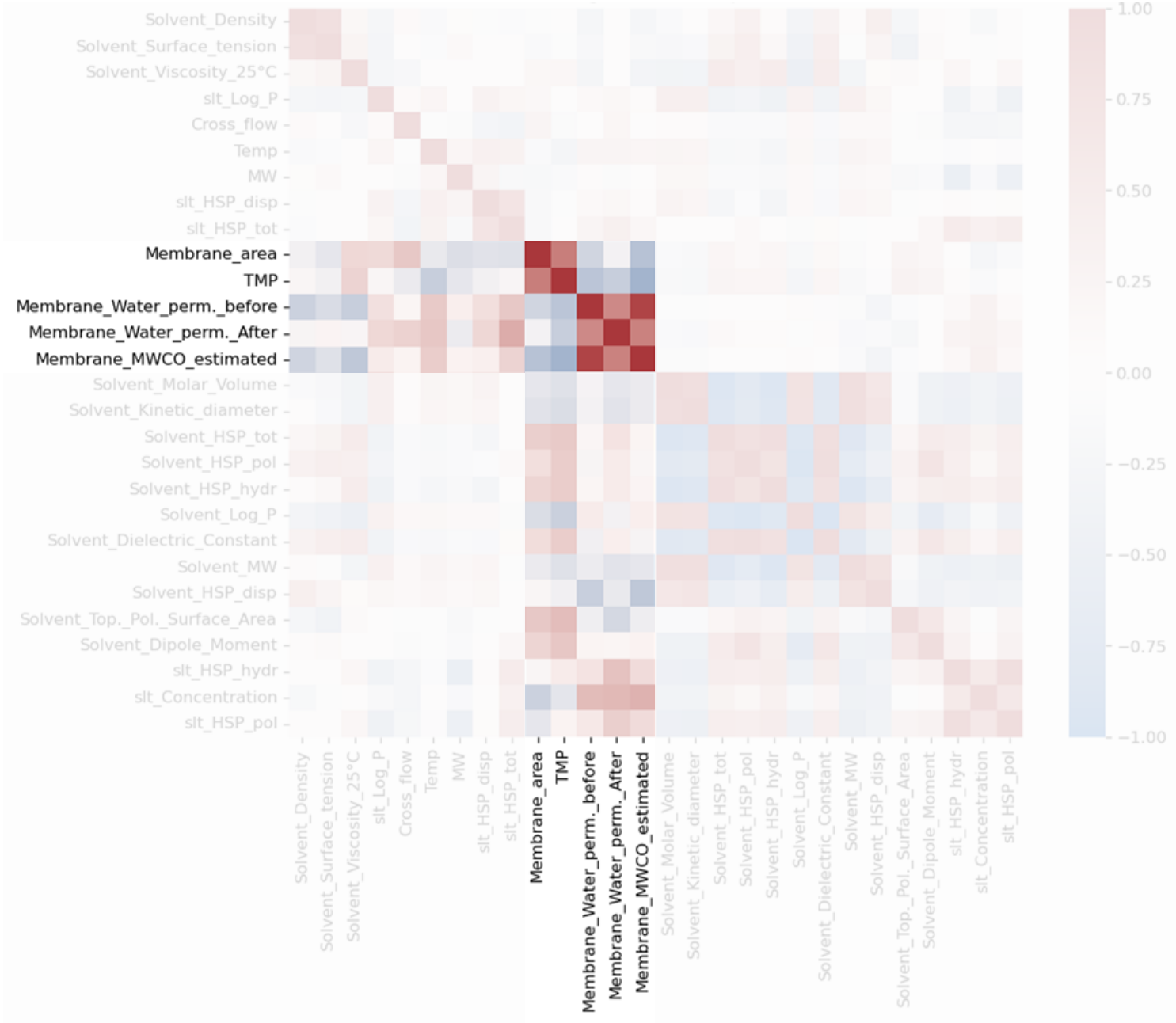
Note Color coding

Correlations among descriptors help us find patterns

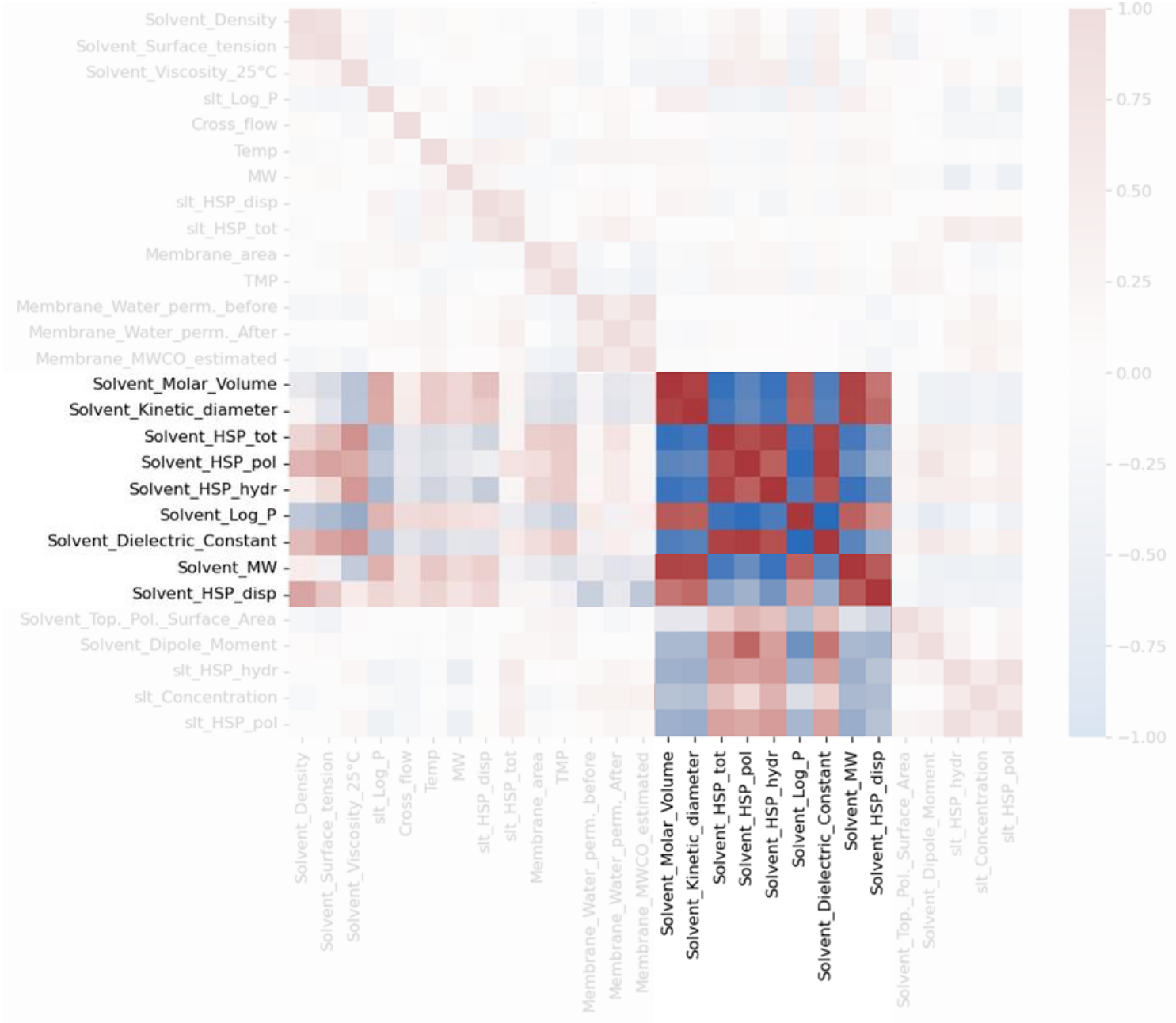
… And provide a global overview of the data of physical properties



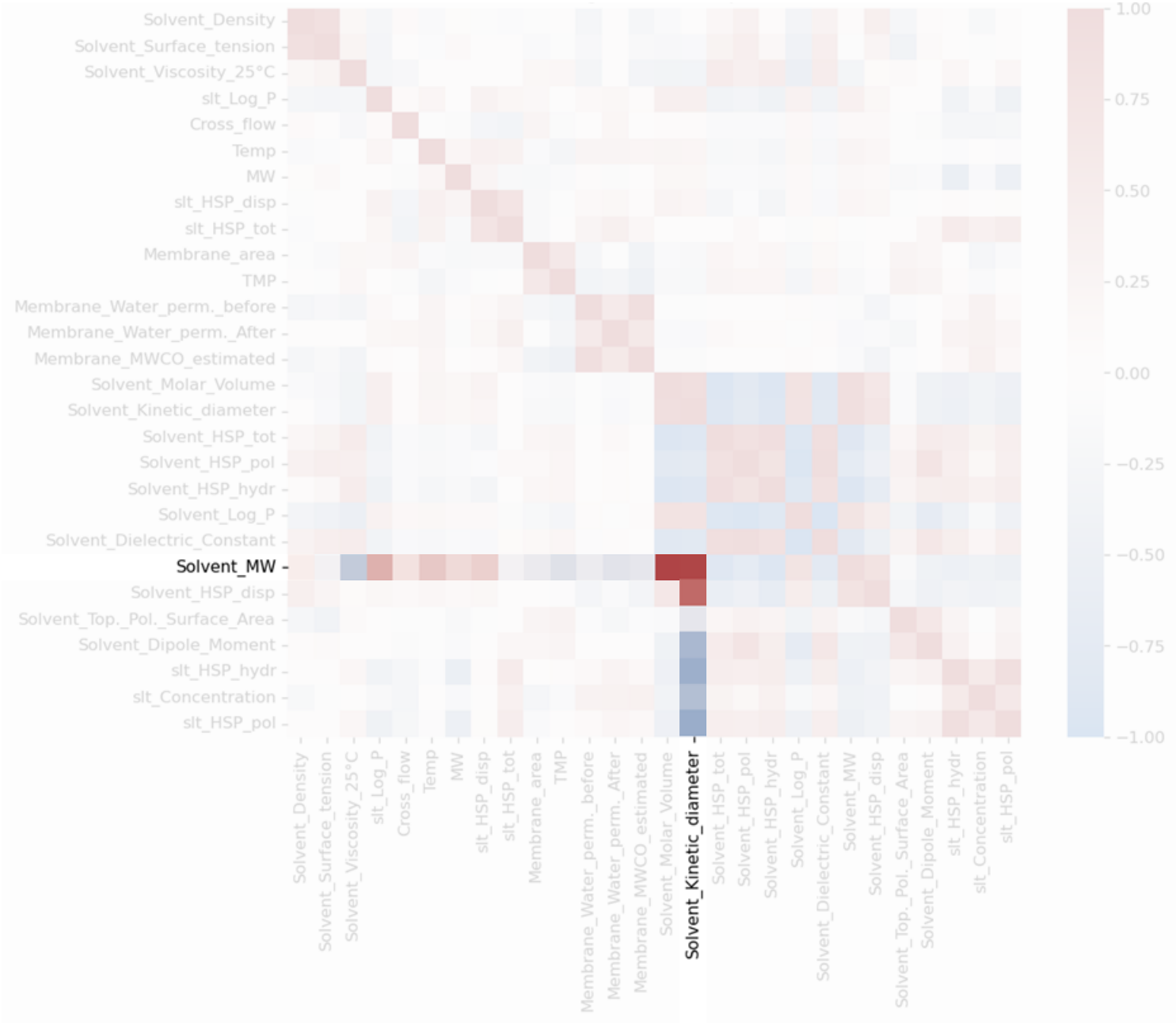
Membrane properties



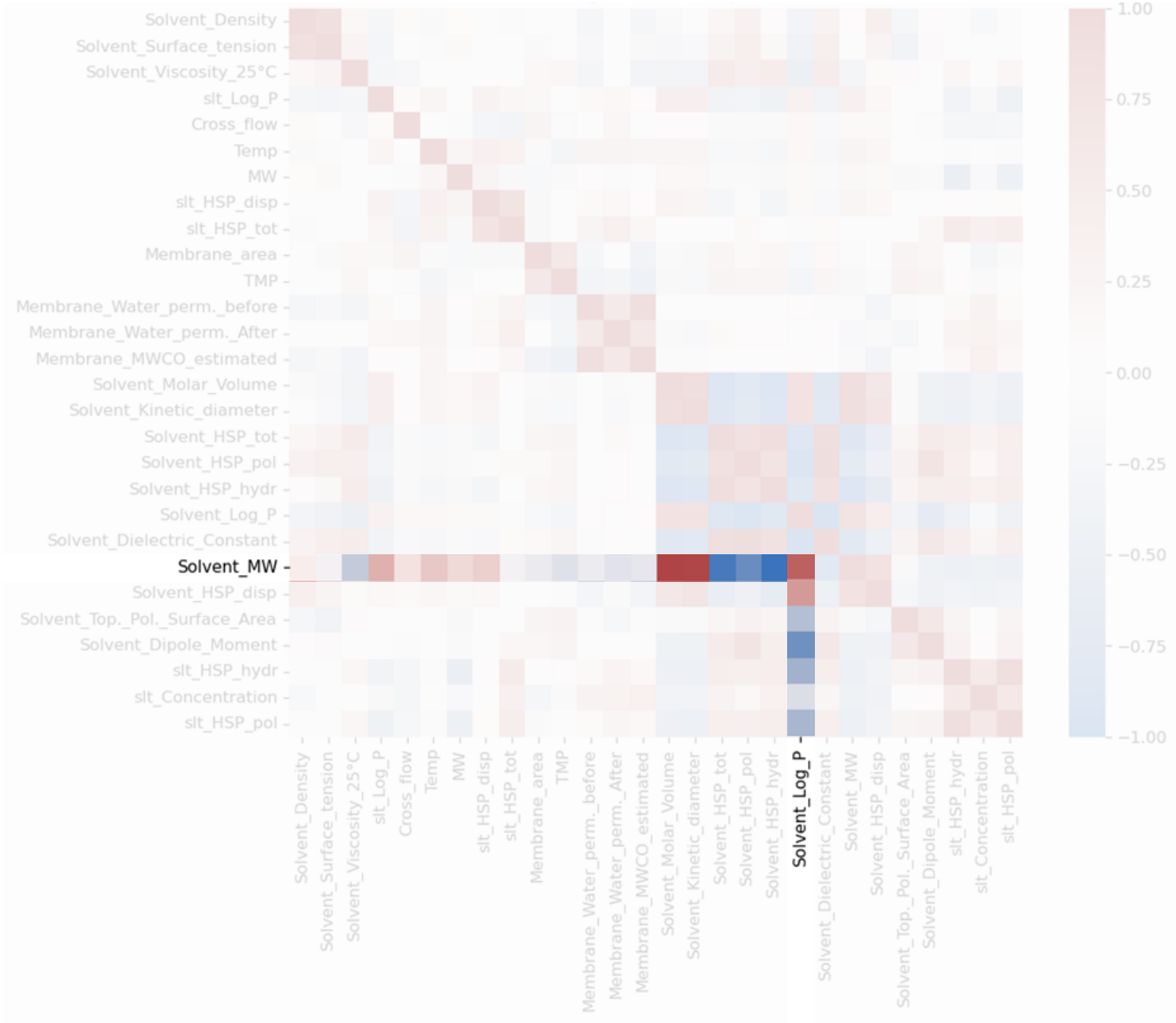
Solvent properties are very noticeably grouped together



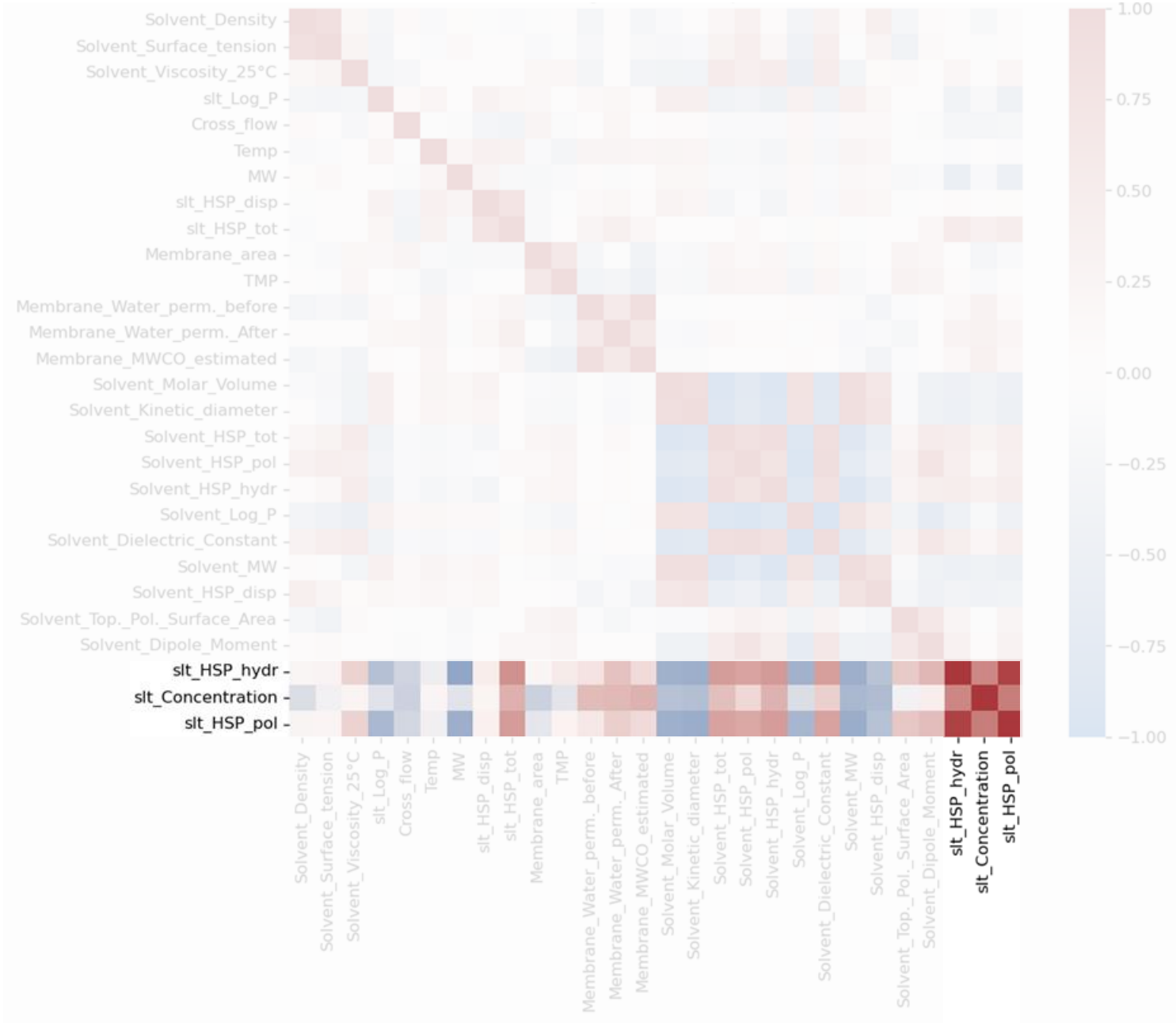
Solvent Molecular weight & Diameter



Solvent polarity and weight

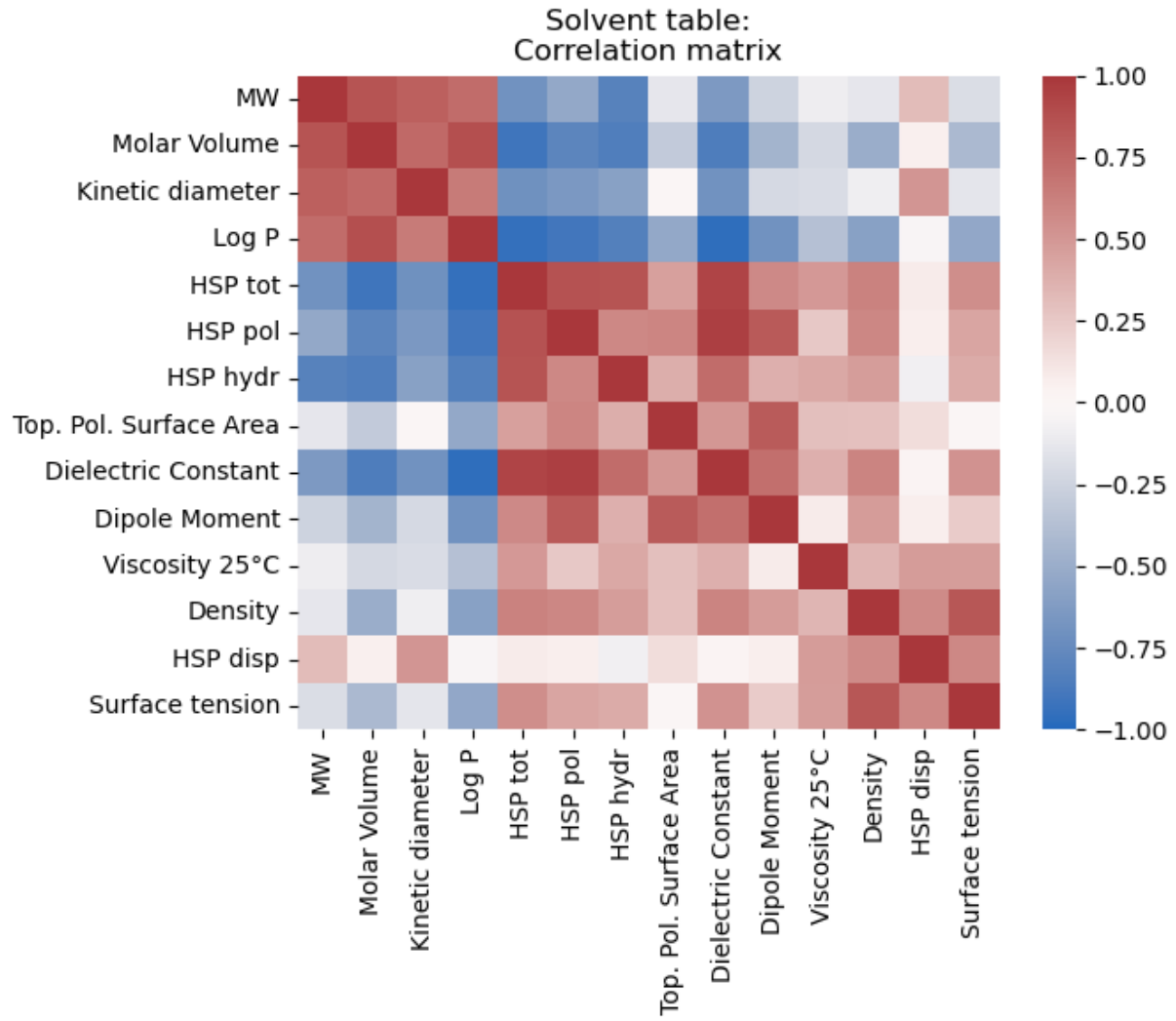


Correlation induced by experimenter



Dimensionality reduction

…of input-space, with minimal loss of information

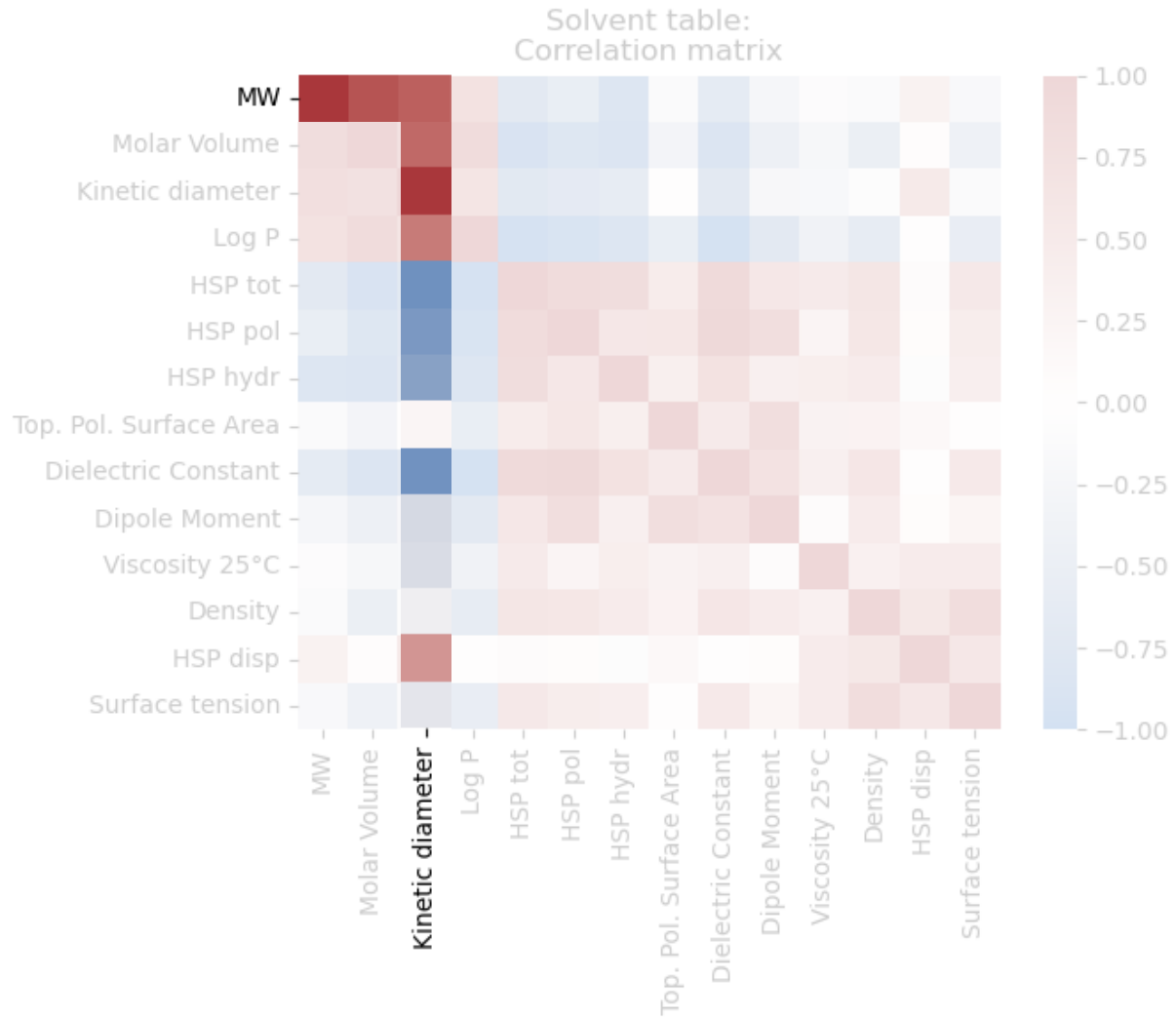


Example for solvent:
Strong correlation between
Molecular weight & Diameter

→ Keep only one without loss of information

Dimensionality reduction

…of input-space, with minimal loss of information



Example for solvent:

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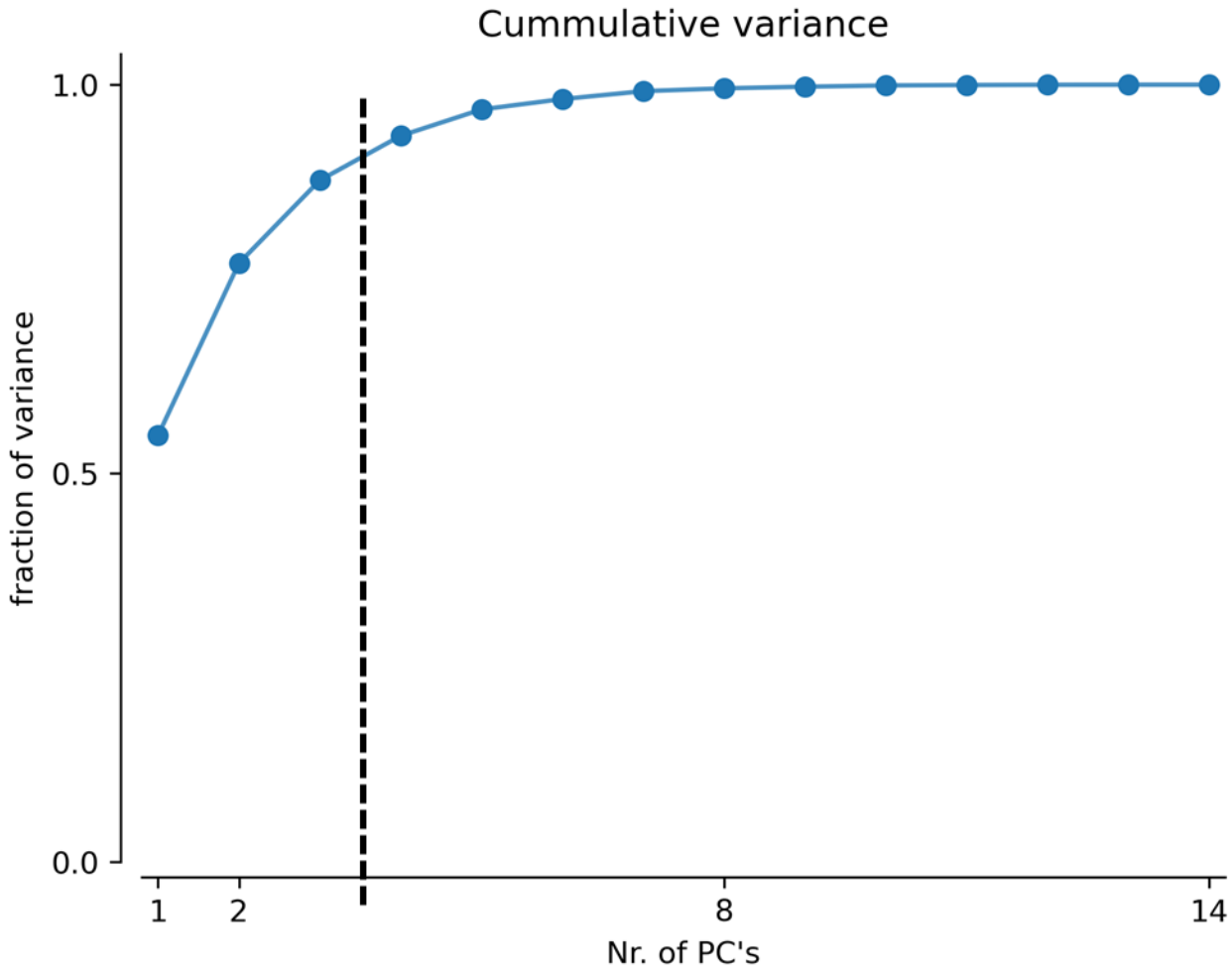
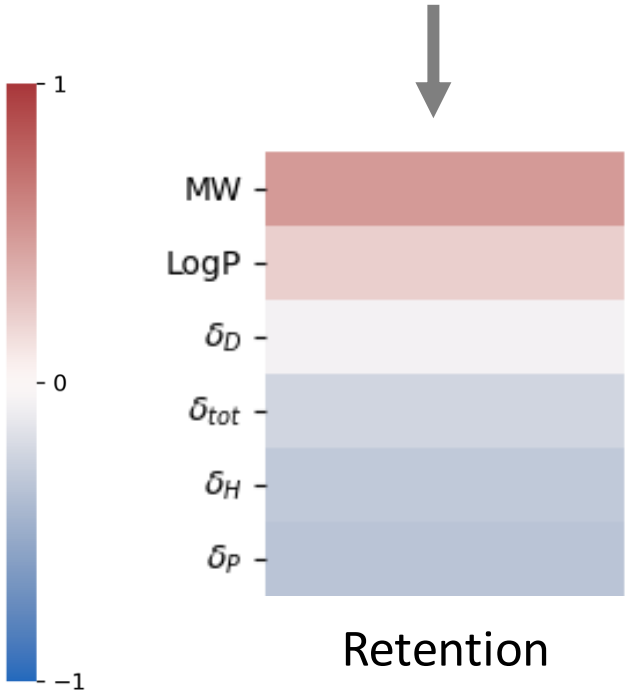
Principle Component Analysis (PCA) to reduce the input dimension



- Using PCA, the solvent can be characterized by only 2 to 4 parameters
- Correct linear combinations found automatically by optimized scripts
- Reduced dimension can be directly fed into data-model

Correlation between descriptors and performance gives physical insight

Solute properties for one native membrane



- Significant correlation between polarity of **solute and retention**
- Expected for a **polar**, native ceramic membrane
- **Interaction** membrane - solute

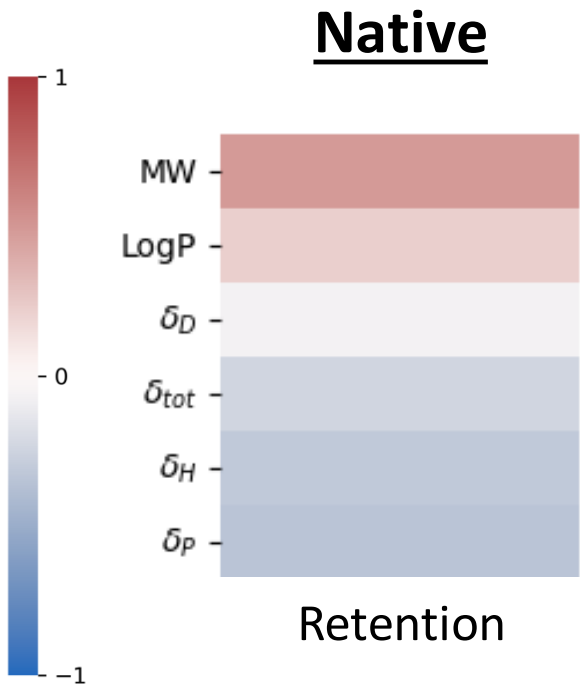
Correlation between descriptors and performance gives physical insight

Grafting

OH → **CH_3**

Decreasing Interactions

Correlation between descriptors and performance gives physical insight



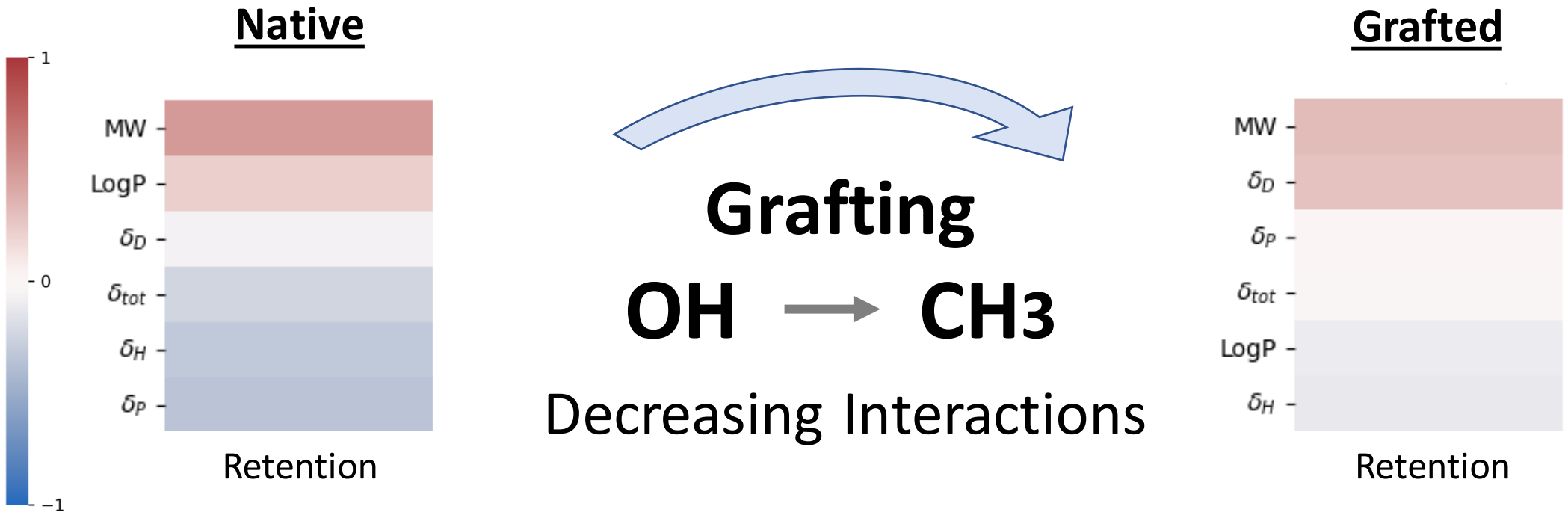
Grafting

OH → CH3

Decreasing Interactions

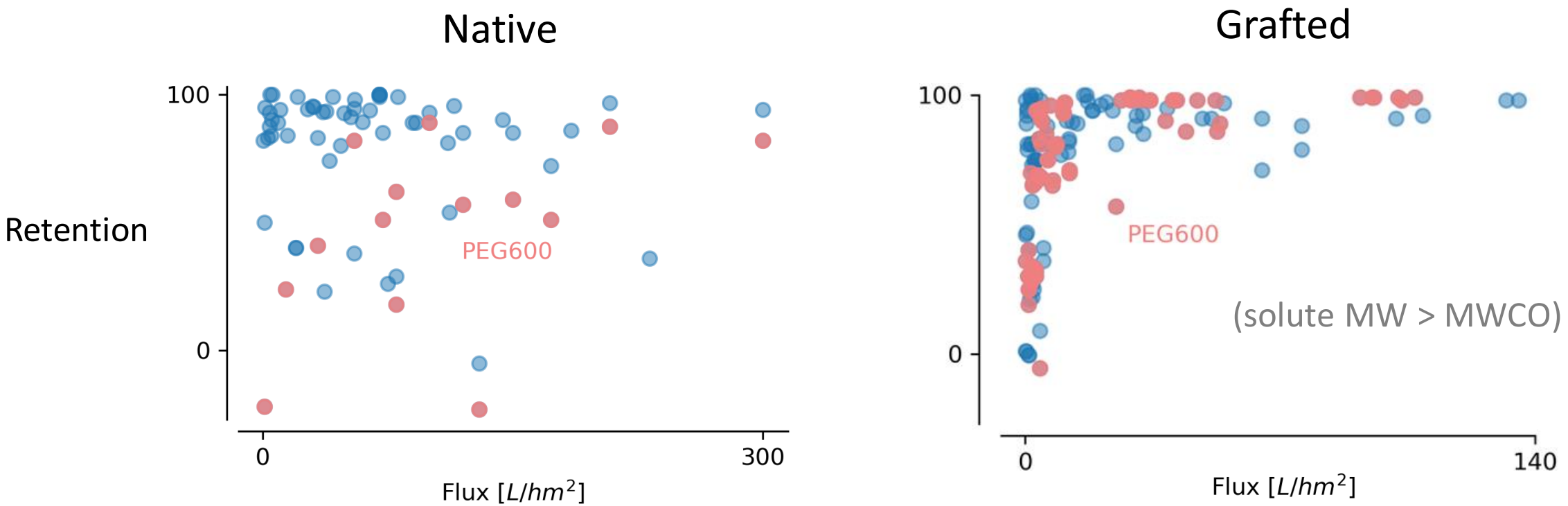
*For a specific membrane: 0,9 nm TiO2 (native & C1)

Correlation between descriptors and performance gives physical insight

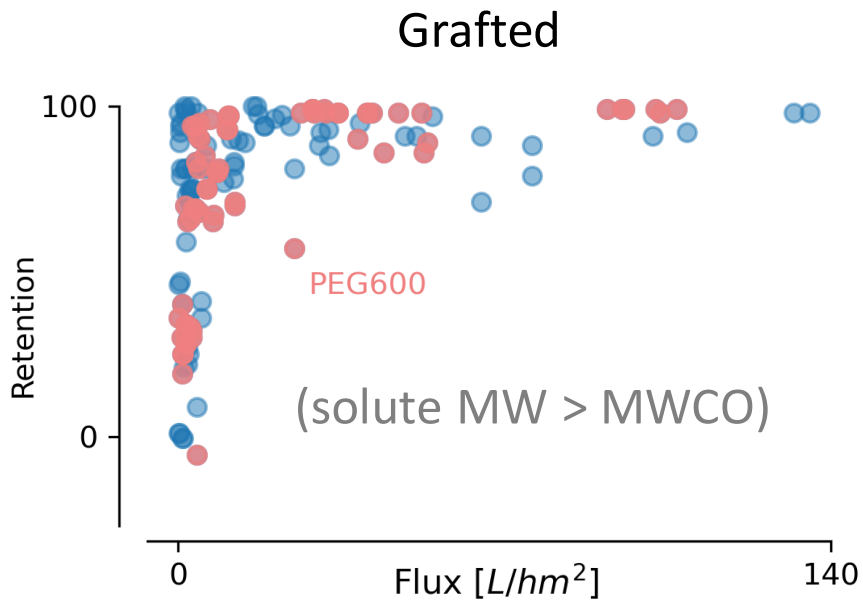


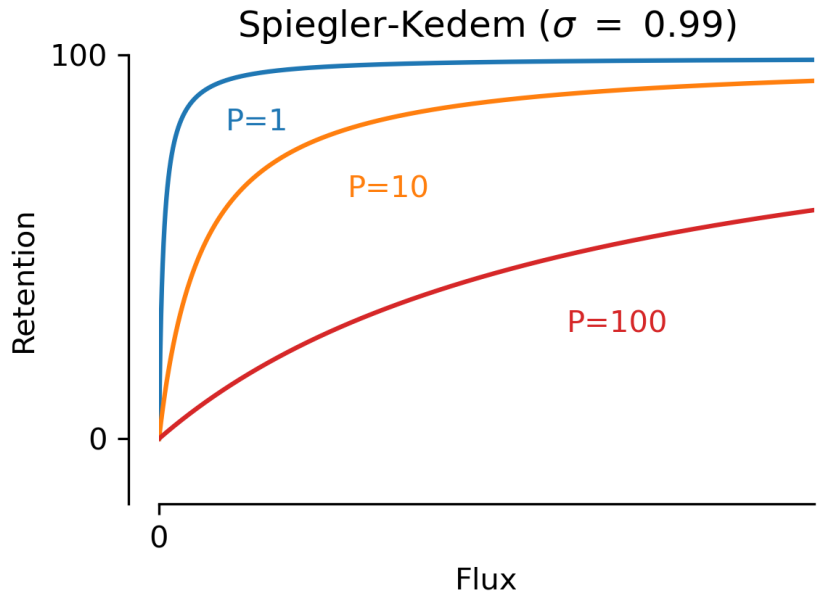
*For a specific membrane: 0,9 nm TiO2 (native & C1)

Retention - Flux curves show remarkably regular behavior



Retention - Flux curves now *do* show similarity to physical model



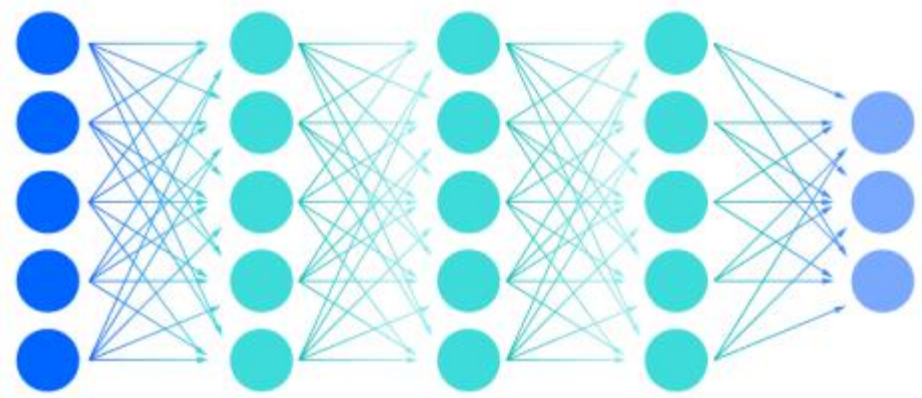


Data-driven models for prediction of membrane performance

Descriptors

Retention
Flux

Descriptors



Retention

Flux

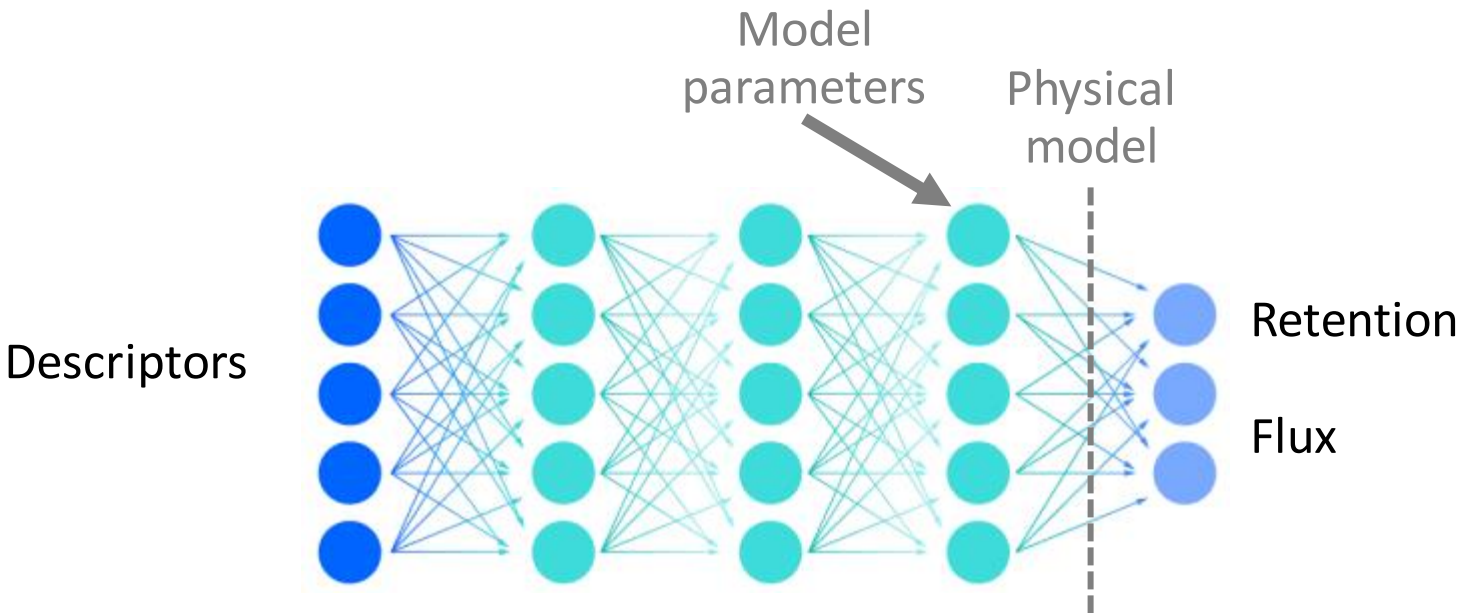
Integrating physics for insight in the mechanism

Descriptors

Physical model

$$R = \left[\frac{1 - e^{-\frac{J(1-\sigma)}{P}}}{1 - \sigma\, e^{-\frac{J(1-\sigma)}{P}}} \right] \sigma$$

Retention
Flux



THANK YOU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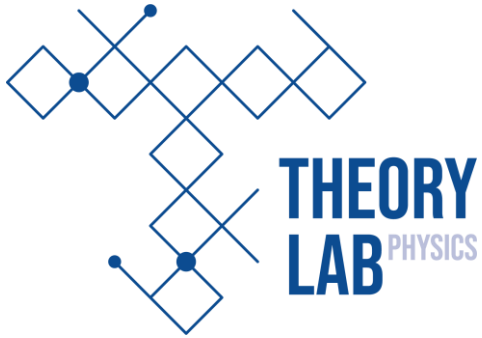
KNOWLEDGE IN ACTION


THEORY
LAB PHYSICS


DSI
DATA SCIENCE INSTITUTE


vito