

PHYSICS-GUIDED NEURAL NETWORKS TO PREDICT CERAMIC OSN MEMBRANE PERFORMANCE

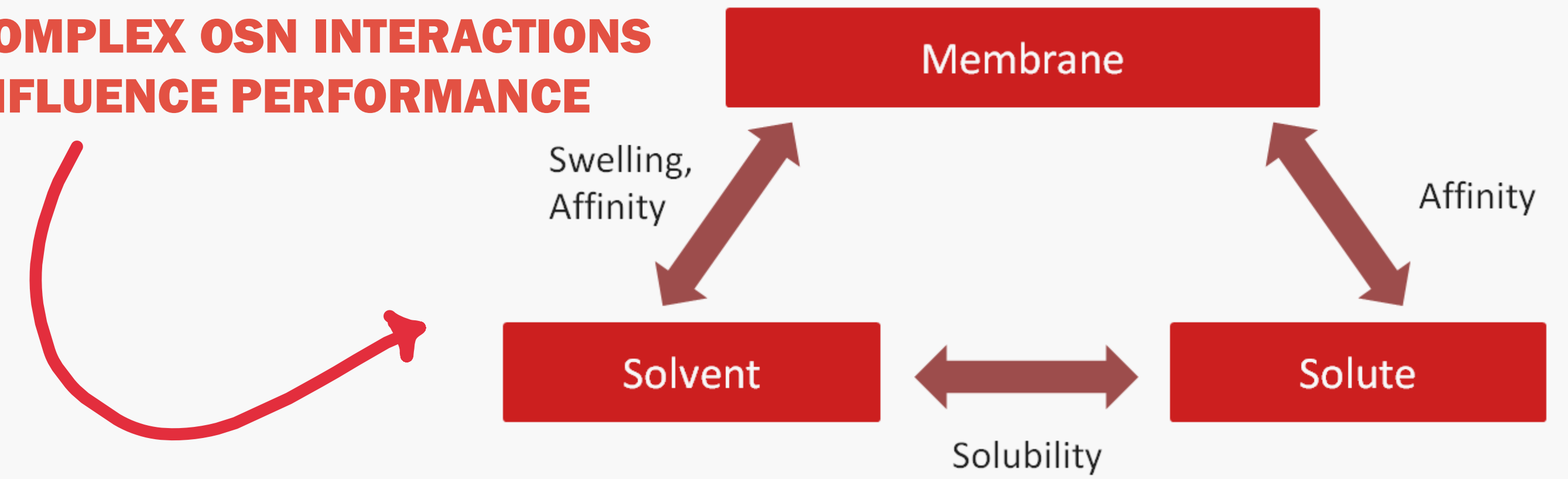
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PREDICTION OF OSN PERFORMANCE IS HARD

Due to the complexity of the membrane separation process, influenced by all mutual solute-solvent-membrane interactions and properties, the **transport mechanism is not well understood**. This leads to a slow, trial-and-error based development process. To **speed up the development process**, and to try and understand the separation mechanism, we resort to **data science**.

COMPLEX OSN INTERACTIONS INFLUENCE PERFORMANCE



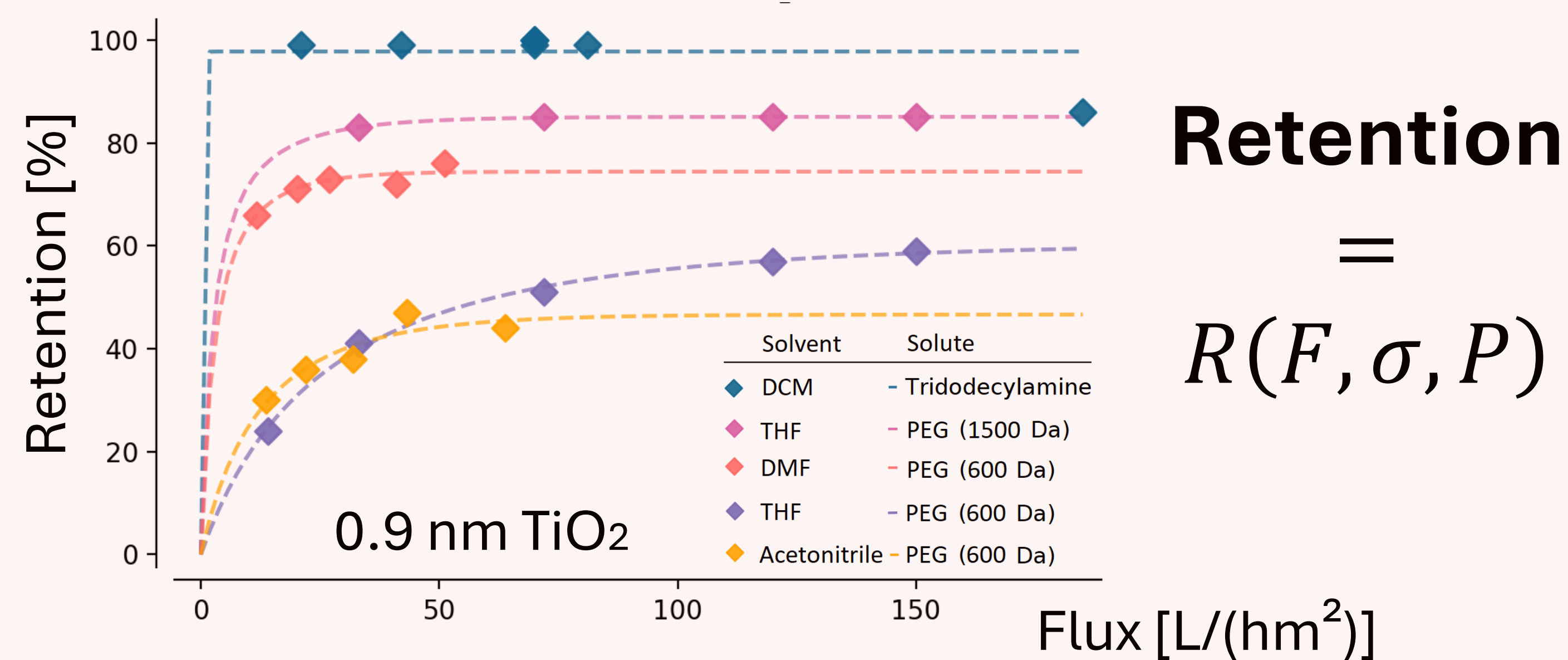
YET, MUCH INVOLVED PHYSICS IS KNOWN

The physics underlying the OSN separation mechanism is generally too complex to build a predictive model. Still, much of the physics is known, although *post factum* used to explain measurement outcomes.

E.g., **Flux scales linearly with transmembrane pressure**:

$$\text{Flux} = F(\sigma, L) = L(\Delta p - \sigma \Delta \Pi),$$

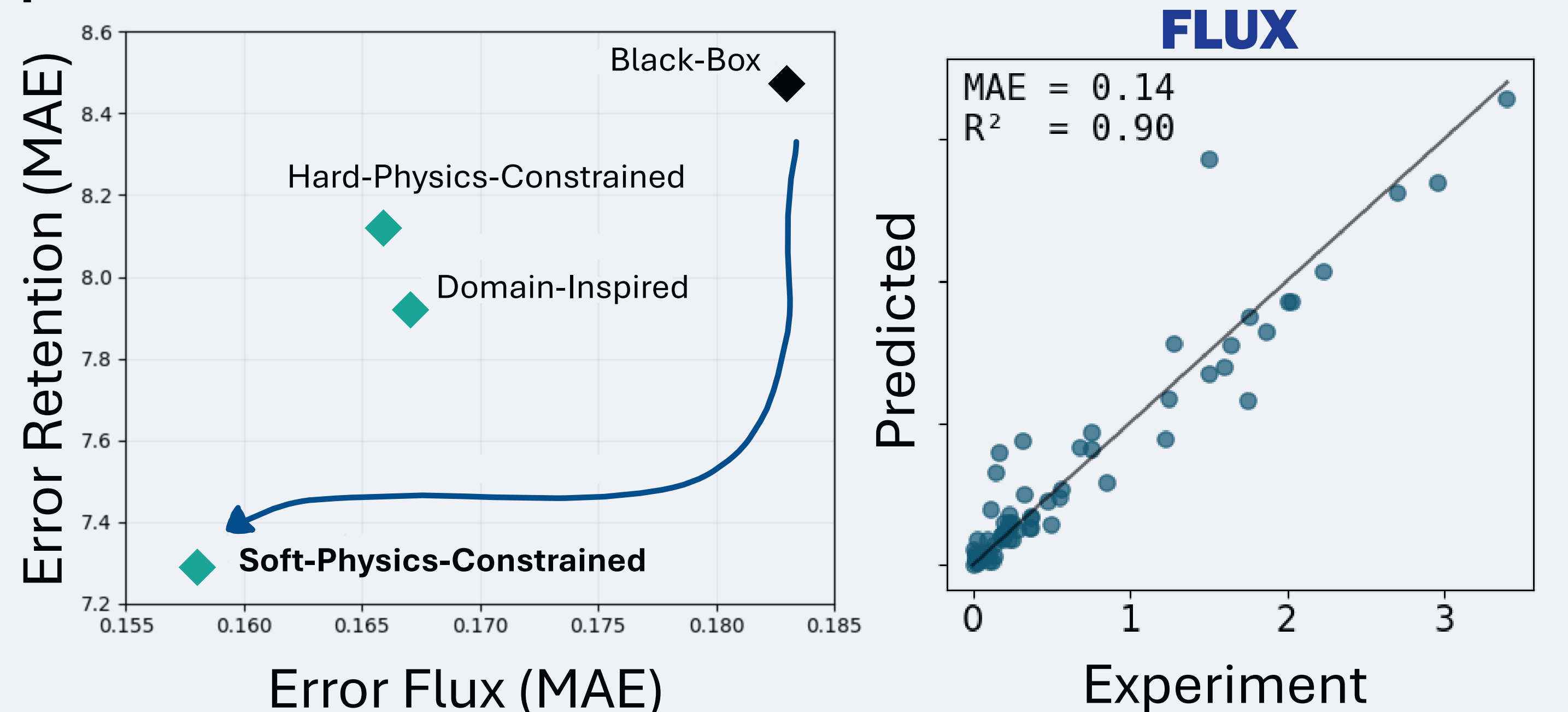
while **retention monotonically increases with flux**, as described by the **Spiegler-Kedem** model:



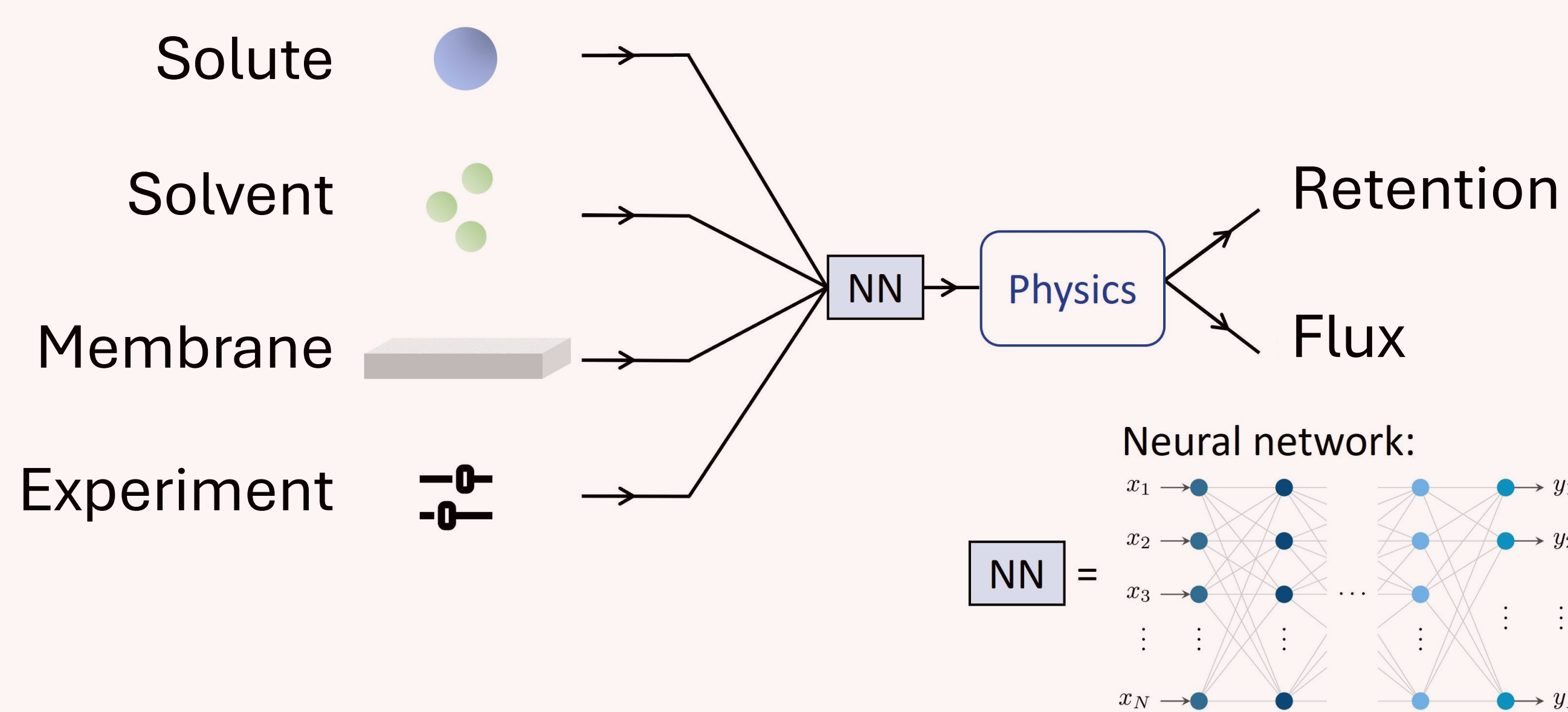
INTEGRATION OF PHYSICS IS BENEFICIAL

Results: Providing the neural net with physical information of any kind improves prediction accuracy and transparency.

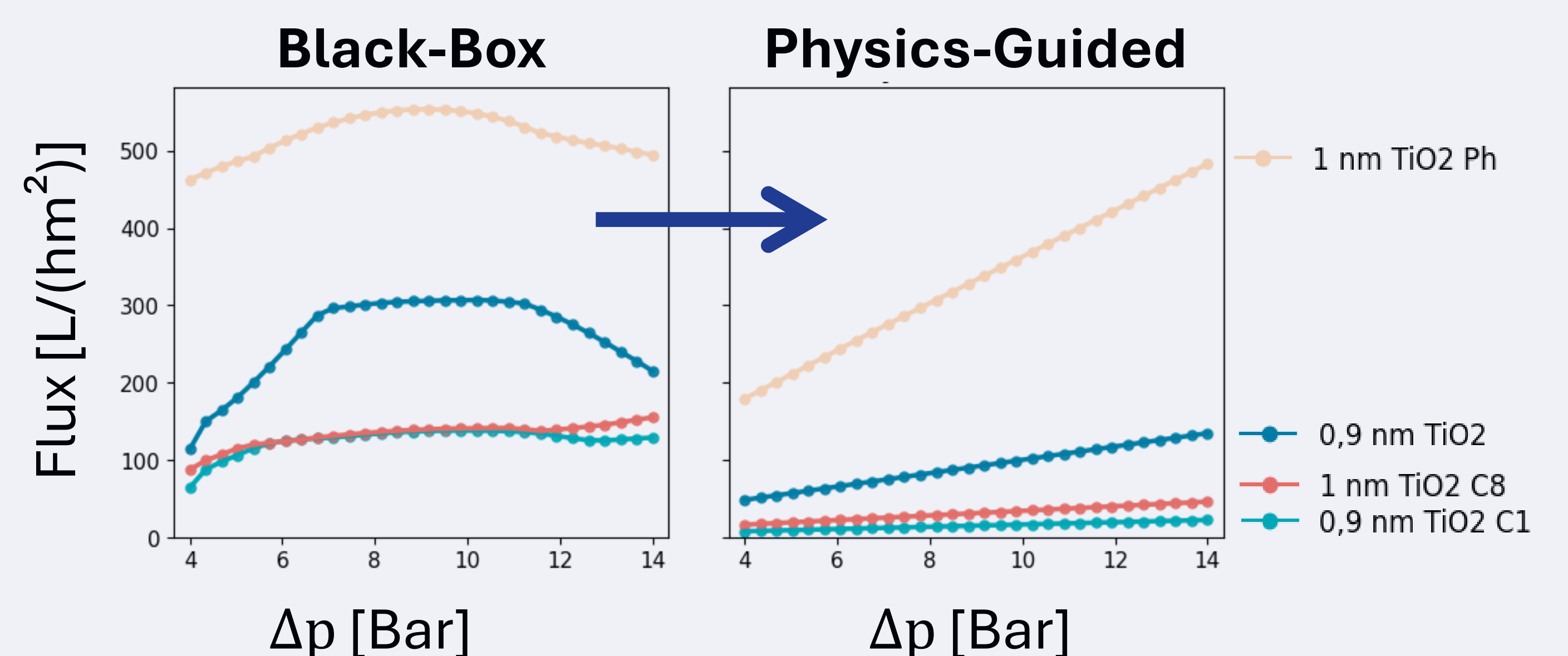
Implementing the **Spiegler-Kedem** is possible: it increases accuracy and provides interpretability, while granting **access to its hidden parameters σ, L and P** .



LET'S EMBED PHYSICS IN A NEURAL NET



PREVENTED UNPHYSICAL HALICUNATIONS



MORE DATA SCIENCE AND MEMBRANES

Review on Data-driven and mechanistic models for OSN. Statistical deep-dive into **native VS grafted membranes**. Using **Solvent HSP and Size**? Care for spurious correlations! **Physics-Guided Neural Networks** (current work).

P.-J. Piccard et al. (2023). *Separations*.
P.-J. Piccard et al. (2025). *Journal of Membrane Science*.
W. Linsen* & P.-J. Piccard* & et al. (2026). *JMS Letters*.
P.-J. Piccard et al. (2026, *In review*).

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