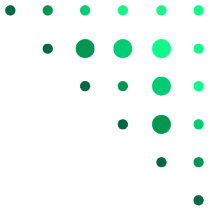


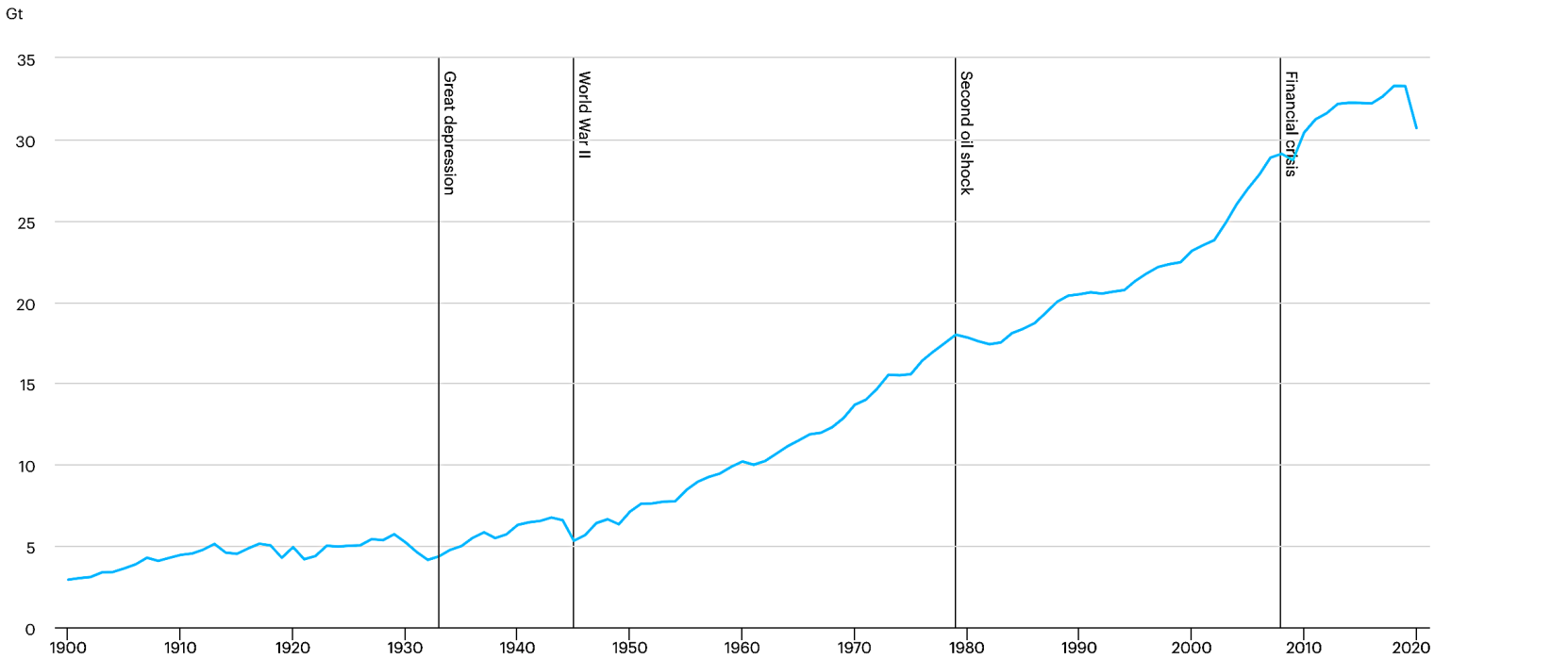
the matter lab

Storing Energy with Organic Molecules: Towards a Metric for Improving Molecular Performance for Redox Flow Batteries

Luis M. Mejía-Mendoza, Martha M. Flores-Leonar, Alán Aspuru-Guzik

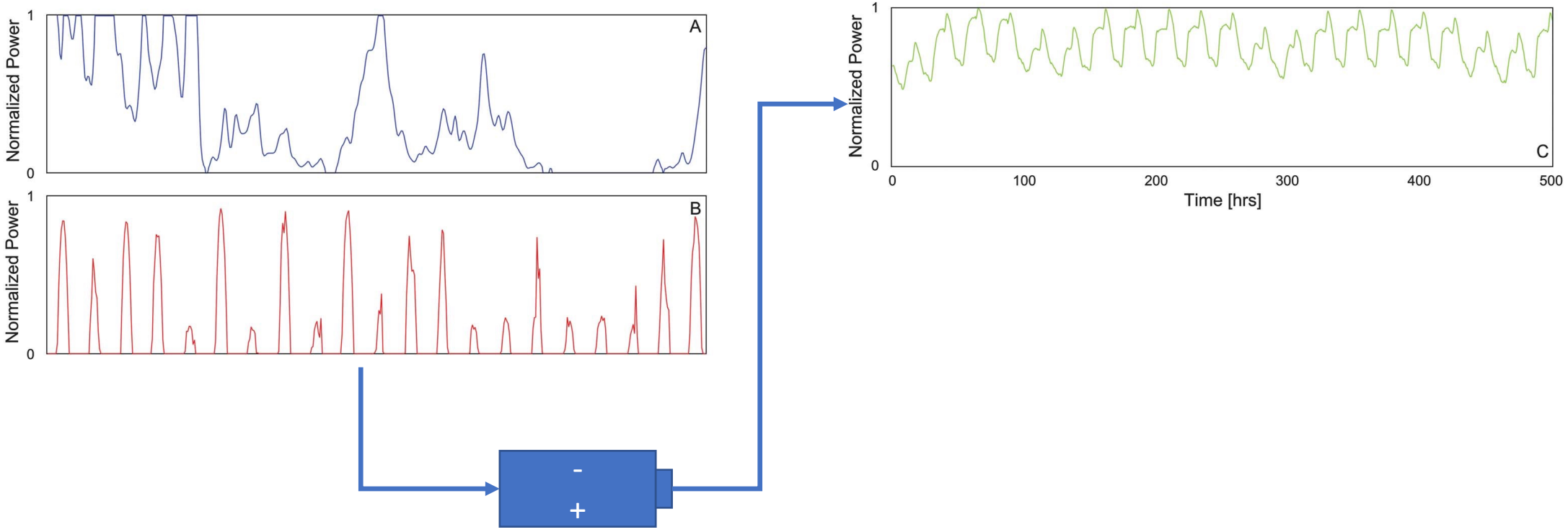
Energy generation, the biggest contributor to CO_2

Global energy-related CO_2 emissions, 1900-2020



Incorporate Renewables to the power grid

Battery storage technology reduce the strain to the power grid due to renewable energy sources



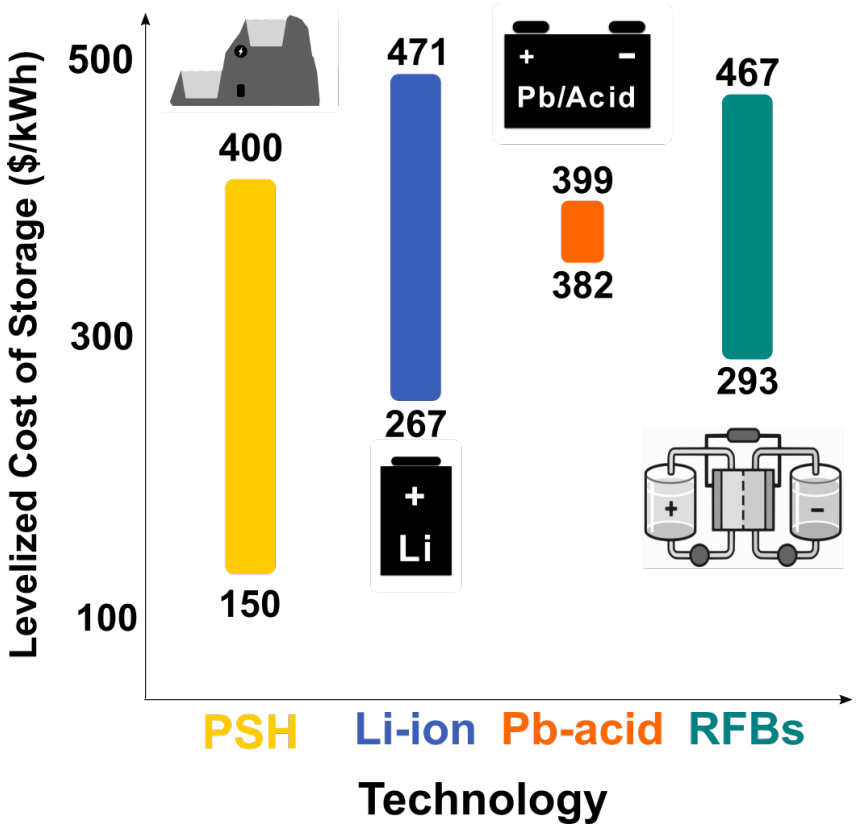
LCOS for different technologies

LCOS of $100/kWh as a target for a storage technology to be commercially viable

$$\textbf{LCOS} \cong \left\{ \frac{\boldsymbol{Sum\ of\ all\ costs \times discount\ rate}}{\boldsymbol{Amount\ of\ electricity\ discharged}} \right\}_{\boldsymbol{year}}$$

LCOS for different technologies

LCOS of $100/kWh as a target for a storage technology to be commercially viable



Cost of a organic redox flow battery

Almost a half of the cost of a Organic Redox Flow Battery (ORFB) are the active materials

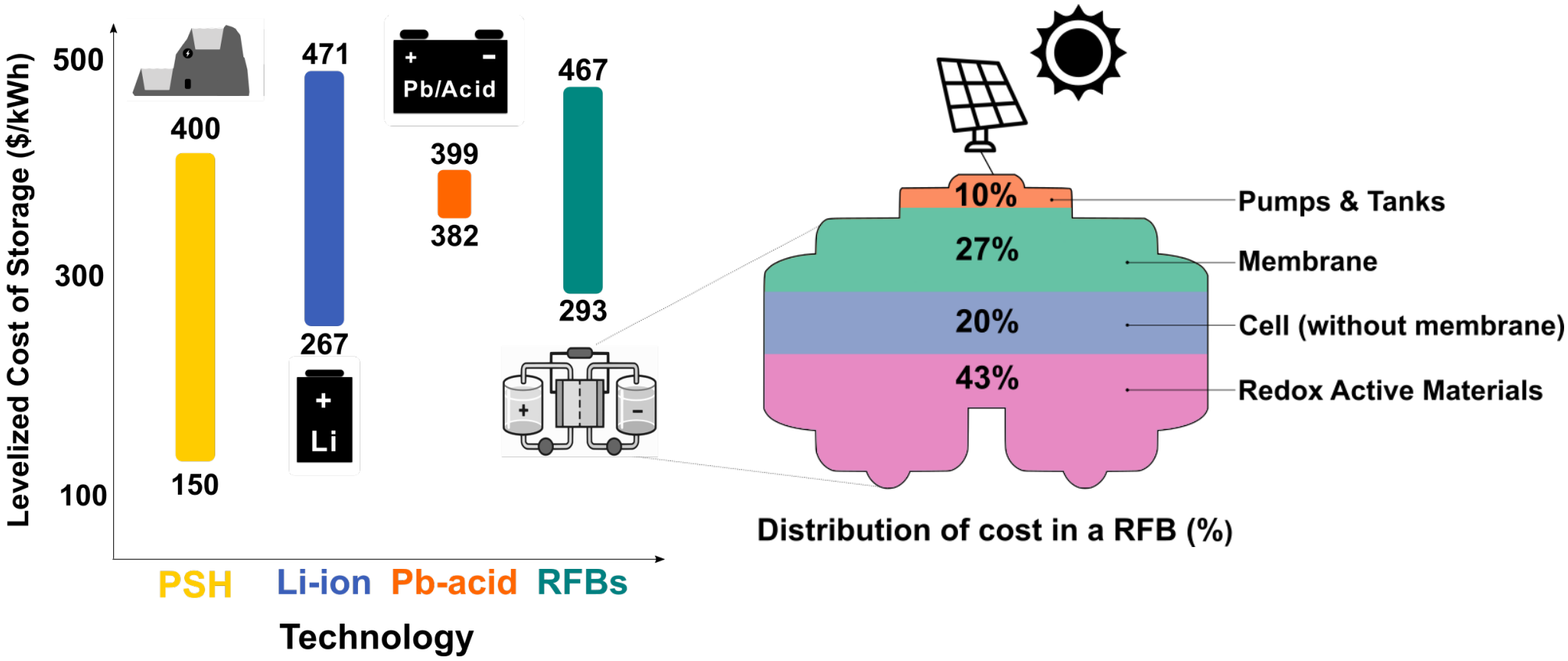
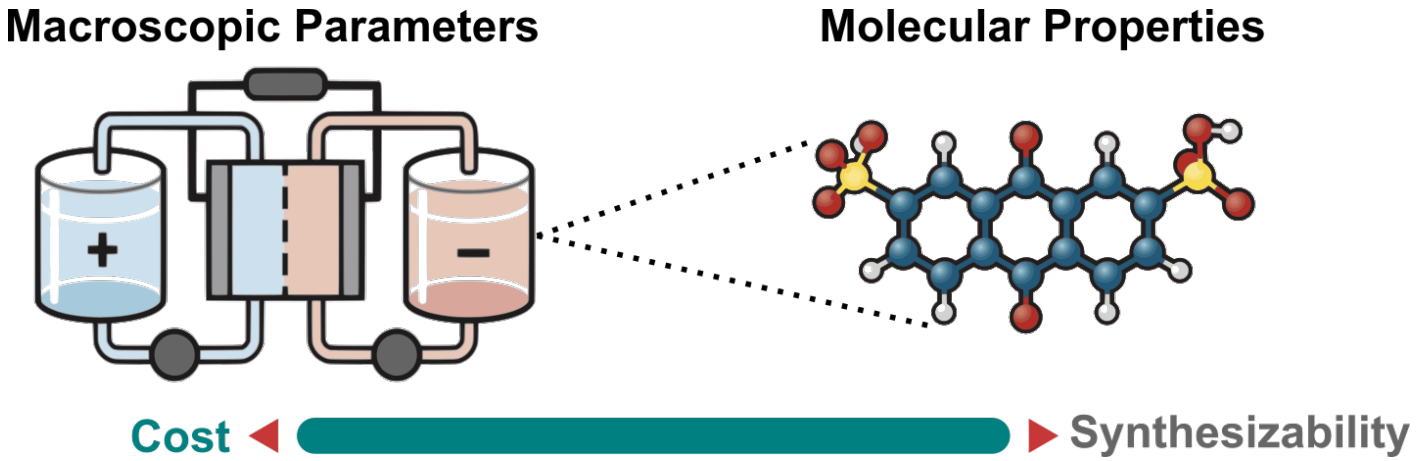
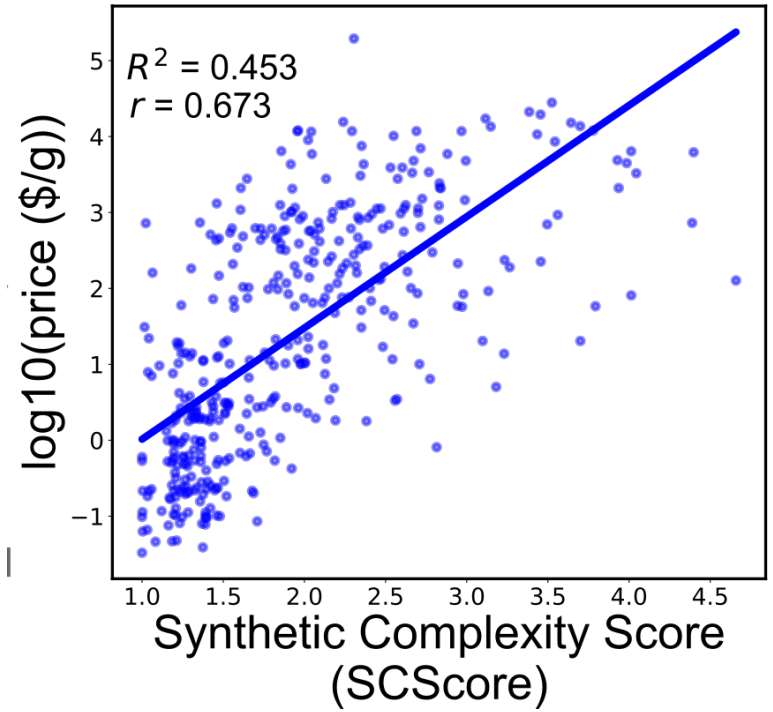


Figure of Merit (FoM) and Cost

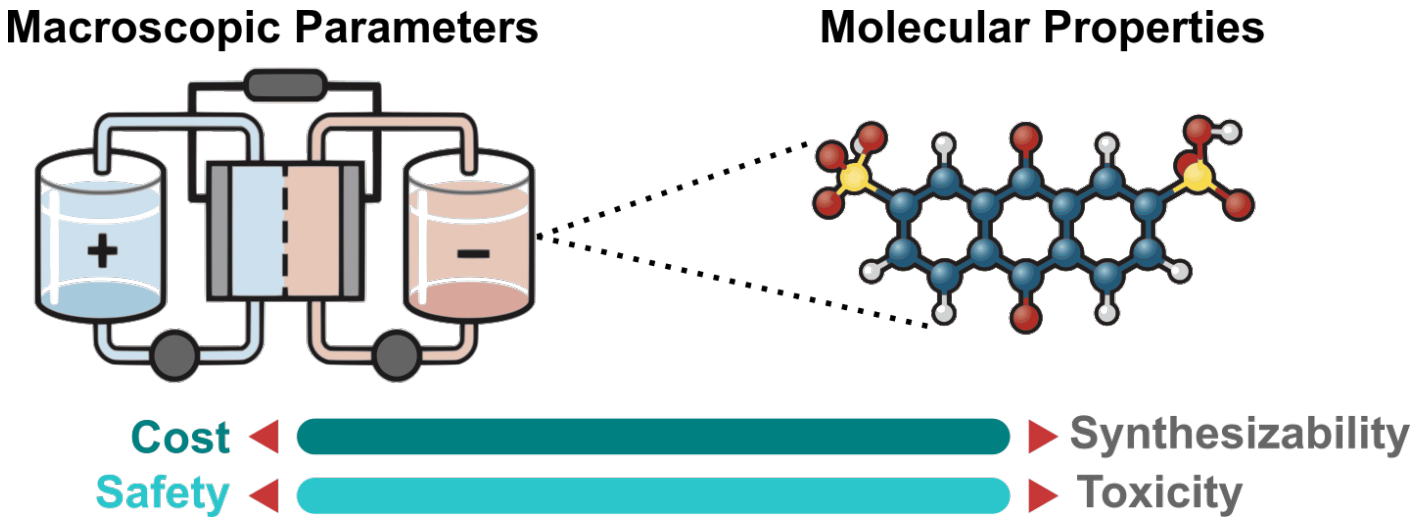
$\mathbf{FoM}(m^+, m^-) = ?$

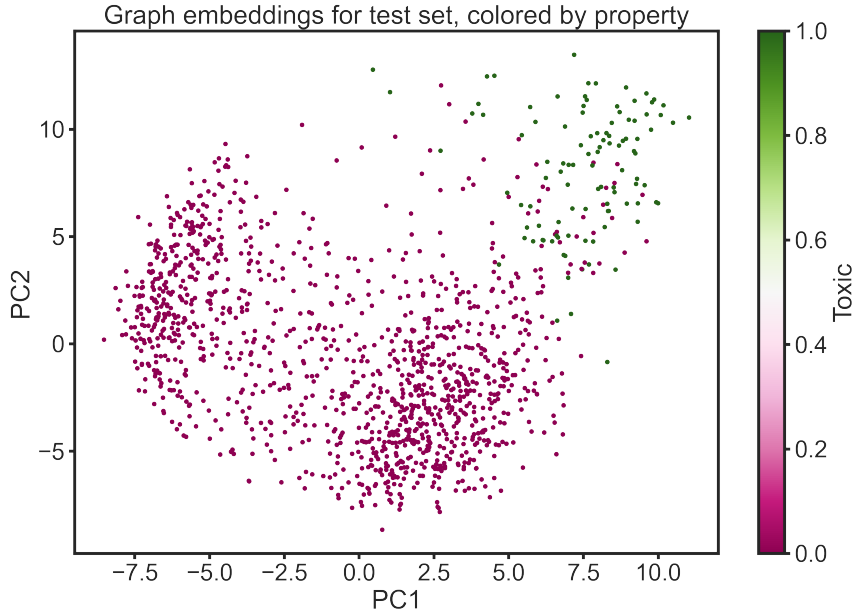




Constructing a FoM

$$\mathbf{FoM}(m^+, m^-) \propto \mathbf{NonToxic}(m^+, m^-)$$

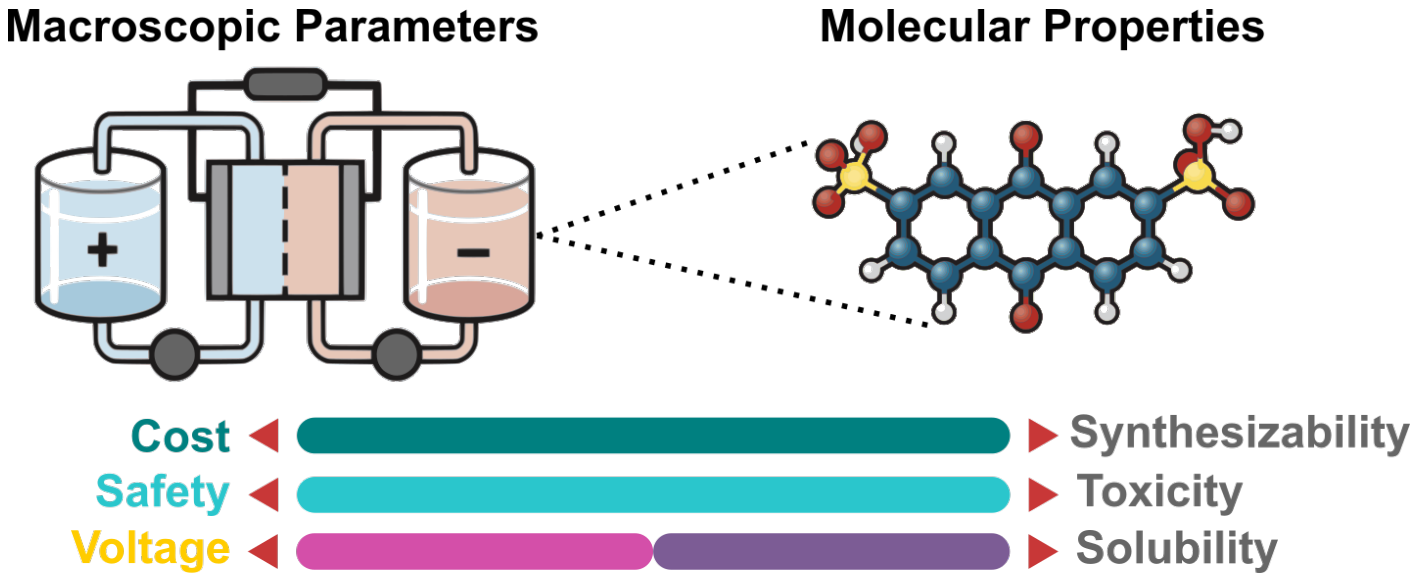


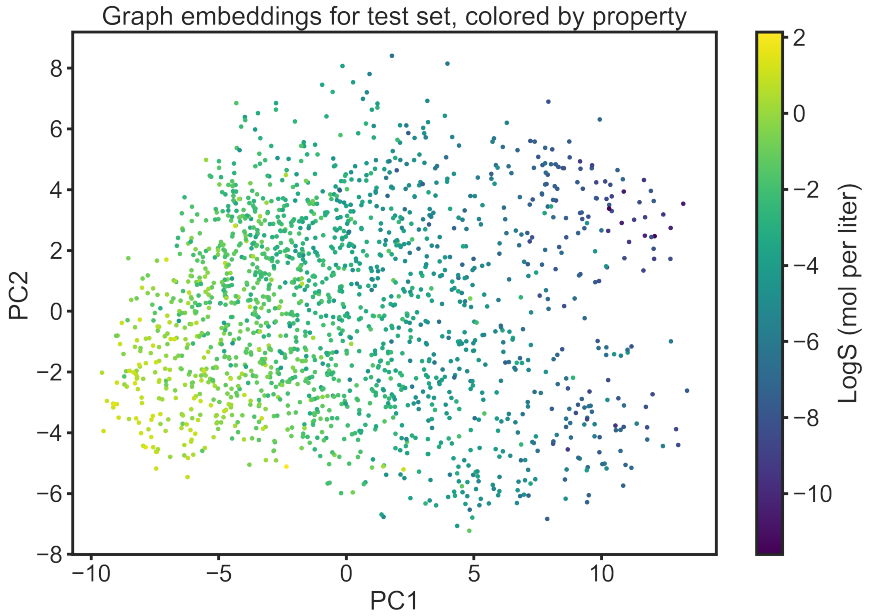


Tox21 dataset

Constructing a FoM

$$\mathbf{FoM}(m^+, m^-) \propto \mathbf{NonToxic}(m^+, m^-) \cdot \mathbf{S}_{min}(m^+, m^-)$$



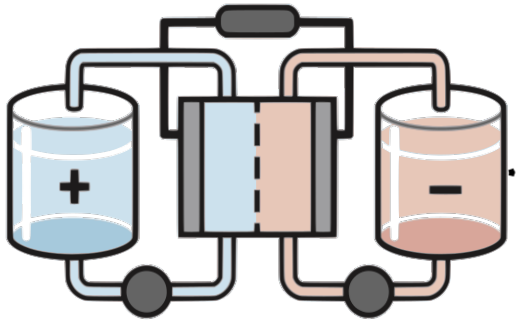


AqSolDB dataset

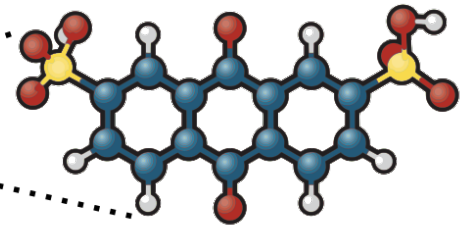
Constructing a FoM

$$\mathbf{FoM}(m^+, m^-) = \mathbf{NonToxic}(m^+, m^-) \cdot \mathbf{S}_{min}(m^+, m^-) \cdot n_{elec} \cdot |\mathbf{ERP}(m^+) - \mathbf{ERP}(m^-)|$$

Macroscopic Parameters



Molecular Properties

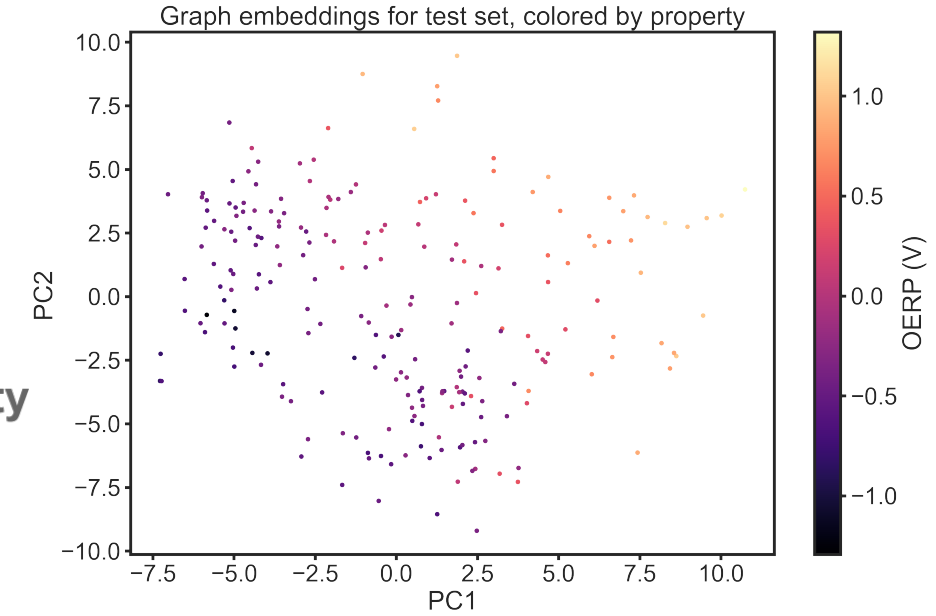


Cost ◀ ▶ Synthesizability

Safety ◀ ▶ Toxicity

Voltage ◀ ▶ Solubility

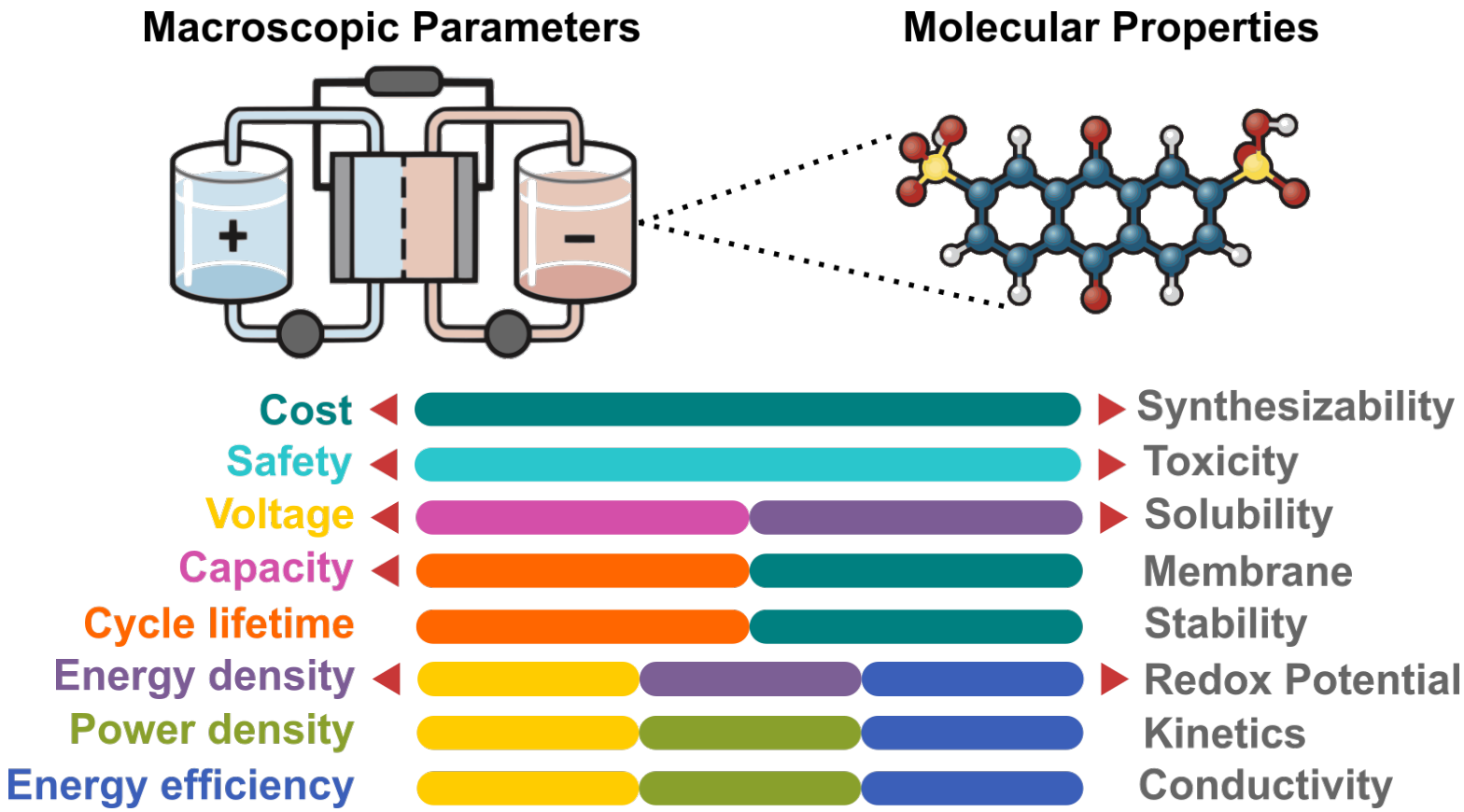
Energy density ◀ ▶ Redox Potential



In-house built dataset

FoM for ORFB

$$\mathbf{FoM}(m^+, m^-) = \mathbf{NonToxic}(m^+, m^-) \cdot \mathbf{S}_{min}(m^+, m^-) \cdot n_{elec} \cdot |\mathbf{ERP}(m^+) - \mathbf{ERP}(m^-)|$$



Areas of opportunity

- Better understanding and modelling of cycle lifetime and kinetics of redox reactions.
- Curation and dissemination of high quality experimental datasets.
- Realization of an autonomous materials platform, that can synthesize and characterize new materials.