# Predicting Transport Properties of Electrolytes for Design of Aqueous Organic Redox Flow Batteries

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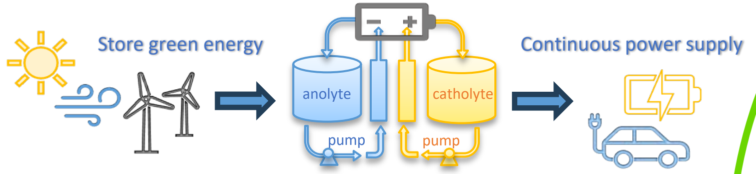
## Introduction

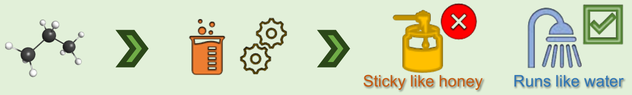
- Fossil fuels cannot keep up with current energy demands without catastrophic consequences to the environment.
- Renewable energy sources, such as wind and solar power, need to be stored when the source is inactive.
- We study aqueous organic redox flow batteries– they are safer than Li-ion or vanadium flow because water is the primary solvent, *making it less toxic, safer to harvest, and cheaper*.
- The electrolyte is pumped in the battery, so viscosity is crucial.




We study the relationship between molecular structure and transport properties to design better electrolytes.

## Research Highlights and Impact

Understand the molecular roots of viscosity to design low-viscosity organic electrolytes.



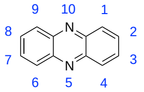

Build bigger, more efficient batteries with long life-time and safety, making renewable energy cheaper and more accessible.

Help keep up with power demands while lowering impact on the environment.

## Materials And Methods

- In a flow battery, the electrolyte is pumped. Optimizing viscosity is crucial to design long-lasting and efficient batteries that will keep flowing.

Use functionalized dihydrophenazine (DHP)



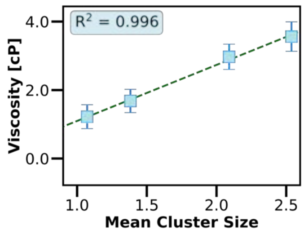

Concentrations: 0.11 M – 1.17 M

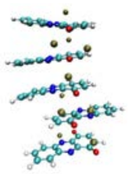
Counterion: $Na^+$, $K^+$ ($Na^+$) ($K^+$)

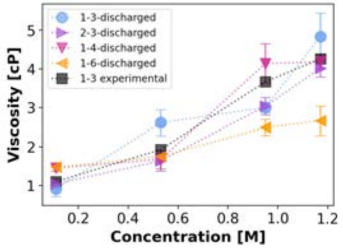
Create DHP variants with different parameters → Run MD simulations with Gromacs → Calculate viscosity using Einstein method → Graph theory-based approach for post-analysis

## Results/Data

- Viscosity increased with concentration but varied depending on variant. We can recreate experimental data well.

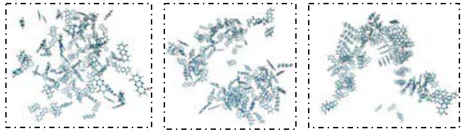




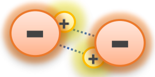

- Viscosity was strongly correlated with size, shape, strength and lifetime of clusters.

Type of clusters formed:



## Discussion/Conclusion

- We can calculate transport properties of electrolytes, even at high concentrations with strong ion-ion interactions.



- The functional group placement in the DHP charge carrier can cause large-scale clustering and aggregation, which impacts viscosity, a key component of flow batteries.
- Understanding the connection between molecular structure and transport properties will help bridge the gap between the electrochemistry of batteries and engineering, combining to build a safe and efficient storage mechanism for renewable energy.

**References:** Hollas, A.; Wei, X.; Murugesan, V.; Nie, Z.; Li, B.; Reed, D.; Liu, J.; Sprenkle, V.; Wang, W., A biomimetic high-capacity phenazine-based anolyte for aqueous organic redox flow batteries. *Nature Energy* **2018,** *3* (6), 508-514.
Wellala, N. P. N.; Hollas, A.; Duanmu, K.; Murugesan, V.; Zhang, X.; Feng, R.; Shao, Y.; Wang, W., Decomposition pathways and mitigation strategies for highly-stable hydroxyphenazine flow battery anolytes. *J. Mater. Chem. A* **2021,** *9* (38), 21918-21928.