Discovery of degradation mechanisms of organic redox flow batteries (RFBs) electrolytes

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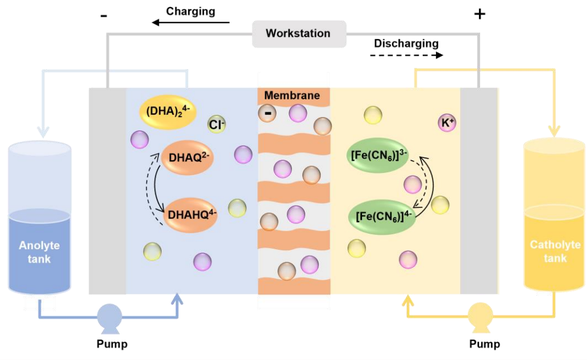
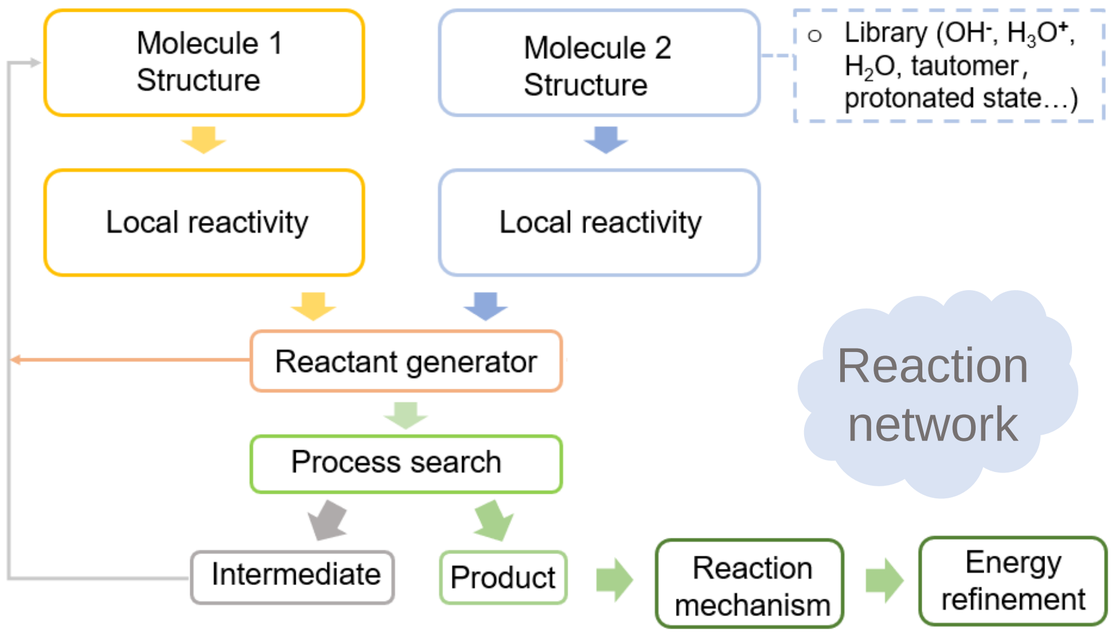
Organic redox flow batteries (RFBs) show great potential for large-scale energy storage, but their thermodynamic chemical instability is a major roadblock. The degradation mechanisms, or even final products, may not be known for new electrolytes, preventing effective mitigation strategies. This project proposes an automated framework to discover the degradation reaction mechanisms RFBs electrolytes, which can be applied to develop new kinetically stable electrolytes with optimized electrochemical properties.

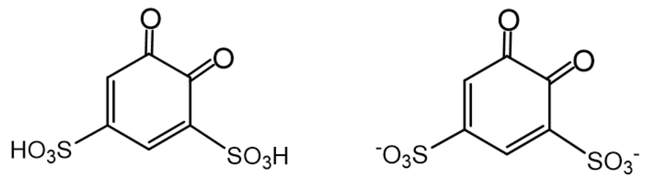


Workflow

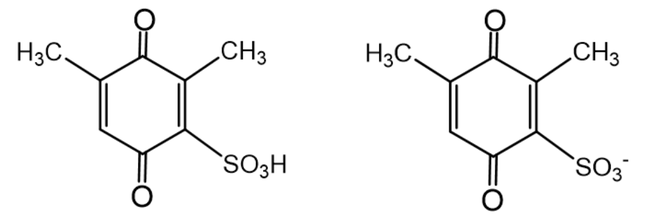


Models

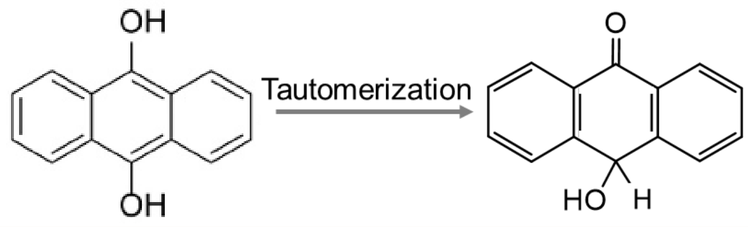
4,5-dihydroxybenzene-1,3-disulfonic acid (BQDS)



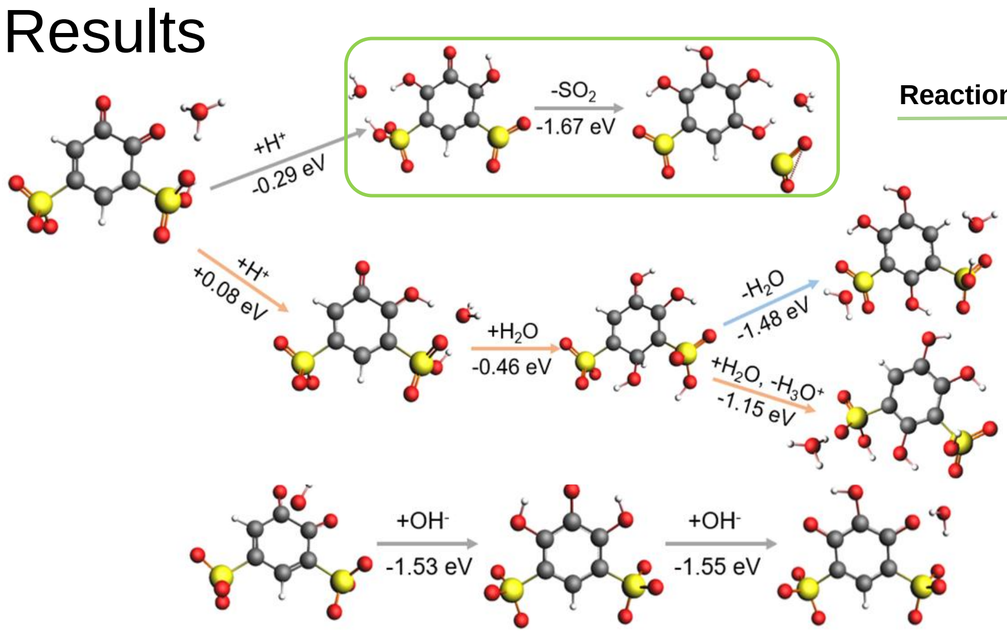
3,6-dihydroxy-2,4-dimethylbenzenesulfonic acid (DHDMBS)



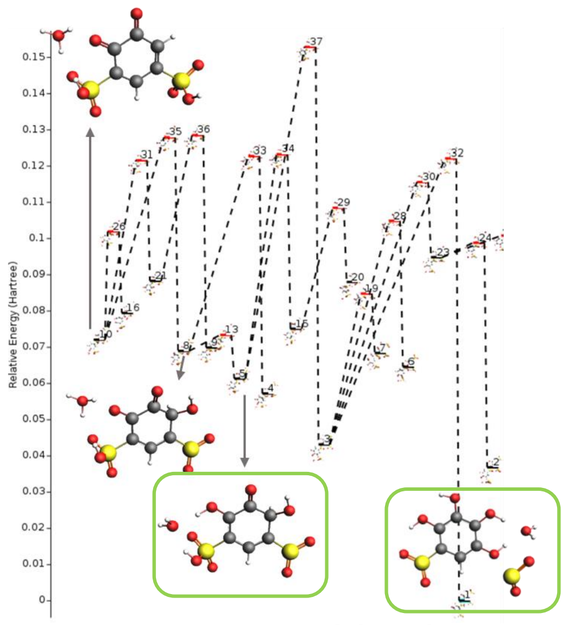
Anthrahydroquinone (AHQ)



Results

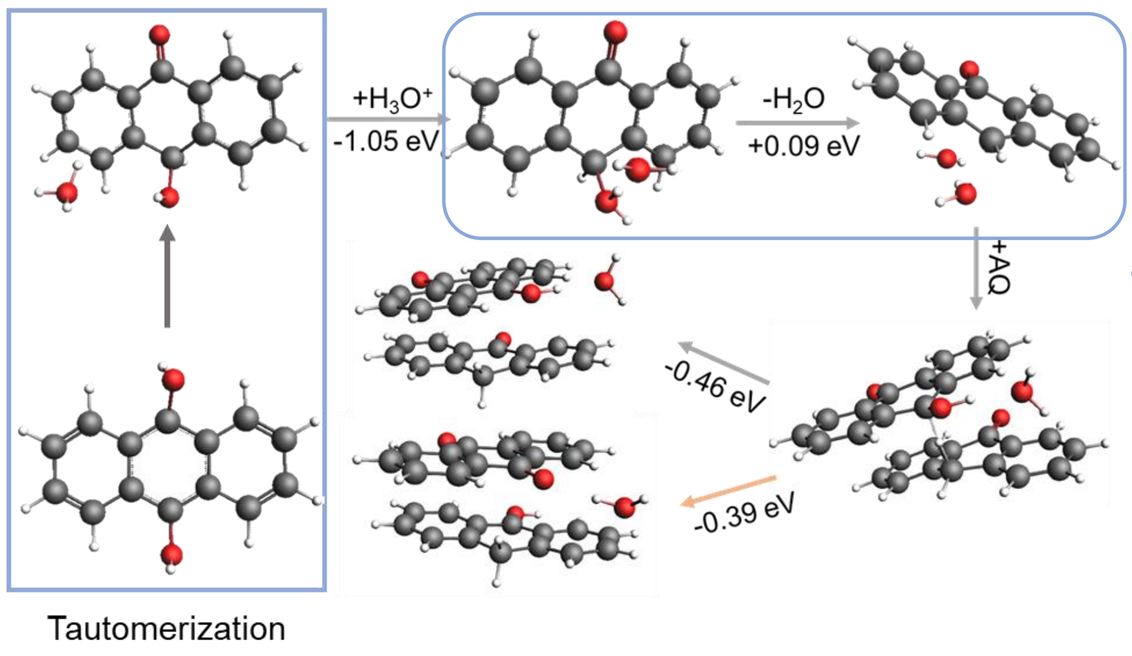


Reaction network

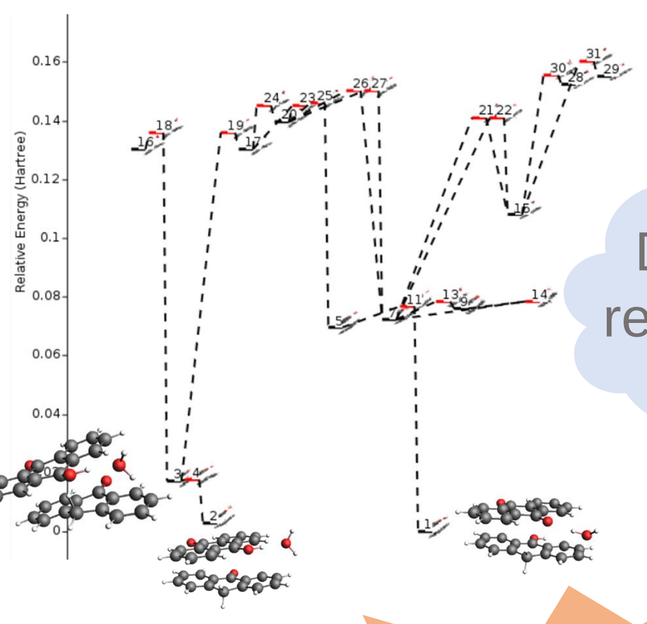


Potential products

Acid-/base-catalyzed degradation mechanism of BQDS



Tautomerization



Disproportion reaction of HAQ

Using our algorithm, we successfully mapped out a full reaction network of

- substituted quinones under acidic/basic conditions
- disproportionation reaction of anthrahydroquinone under acidic condition.

Discovering new degradation mechanisms…

References

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