Iron Complexes with Sugar-Derived Ligands for Aqueous Flow Batteries

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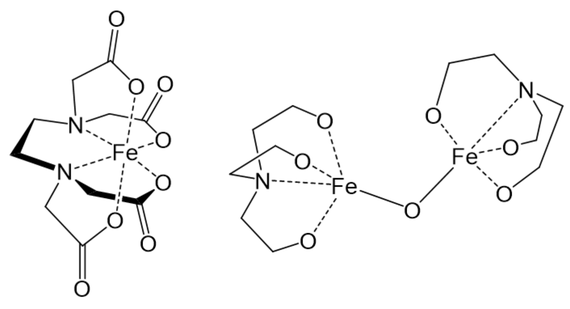
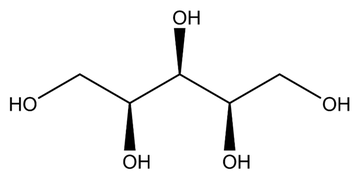
Introduction

Transition metals
- Fe, Cu, Co, Mn…

Organic ligands
- TEA, EDTA, PDTA…

Metal-Organic complexes

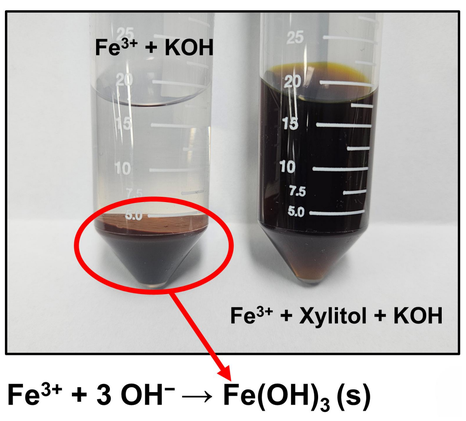




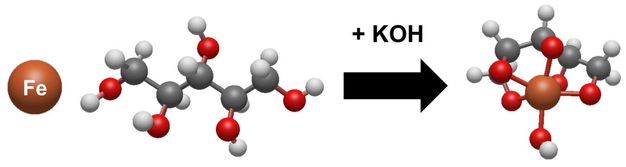
Xylitol

- Iron-based complexes are suitable active materials for flow batteries (FBs) due to their low cost and abundant resources.
- However, the high cost of ligands and the dependence on nitrogen-containing ligand structures limit the development of diverse iron-based complexes.
- This study introduces xylitol as a nitrogen-free ligand to develop a new iron-organic complex, Fe(Xylitol), for application as an active material in FBs.

Result and Discussion



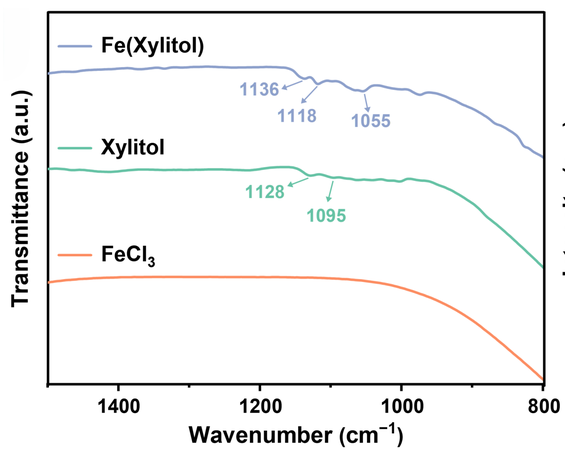
$Fe^{3+} + 3\ OH^- \rightarrow Fe(OH)_3\ (s)$

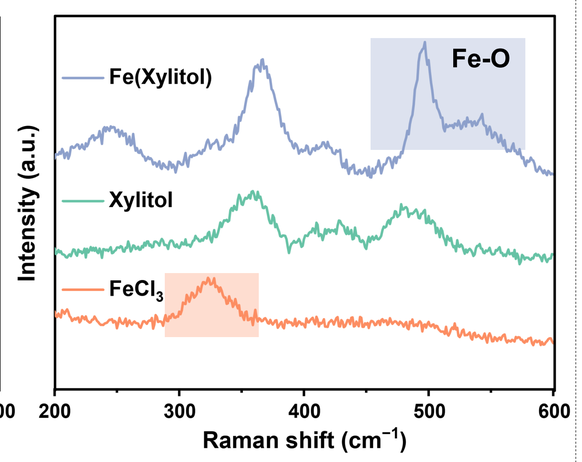


	DIPSO	BIS-TRIS	Xylitol
Price of materials ($ mol^{-1}) *	502.37	124.78	**21.98**

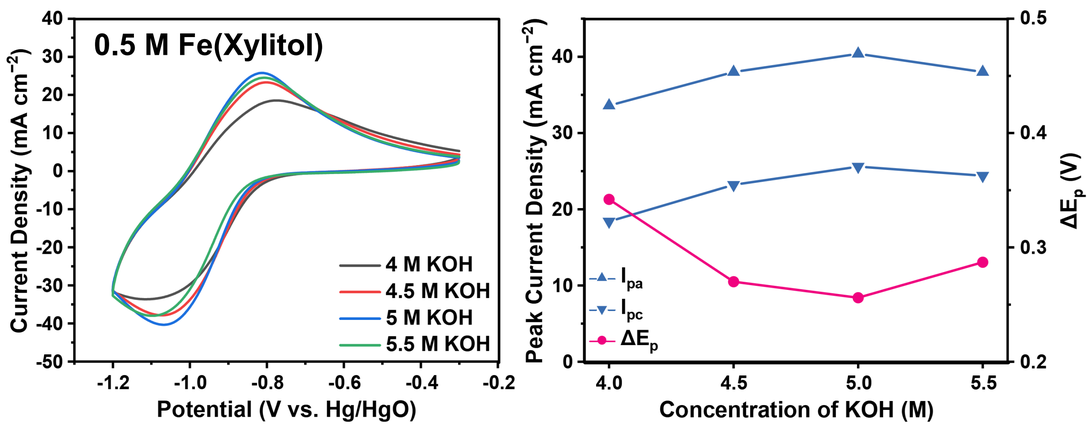
* The cost of chemicals was surveyed at webpages of Thermofisher Scientific at the largest volume in stock [https://chemicals.thermofisher.kr/, last visited on 16th April. 2026]

- Xylitol effectively coordinates with Fe^{3+} under alkaline conditions, suppressing the formation of insoluble $Fe(OH)_3$ precipitates.
- In addition, xylitol offers a significant cost advantage over conventional ligands such as DIPSO and BIS-TRIS.

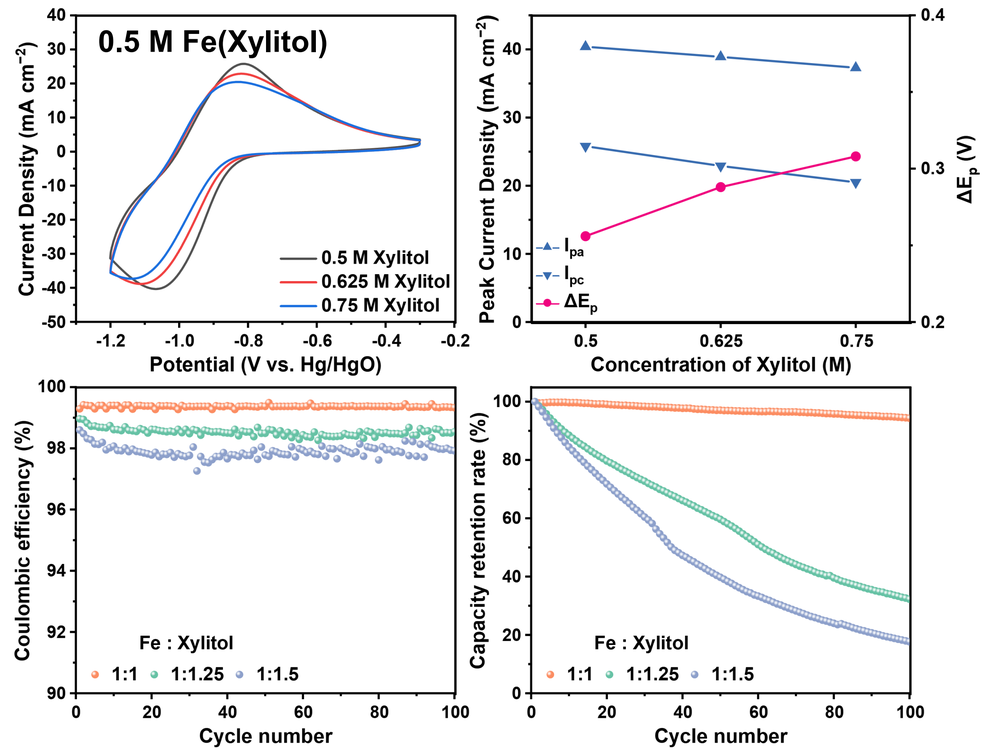




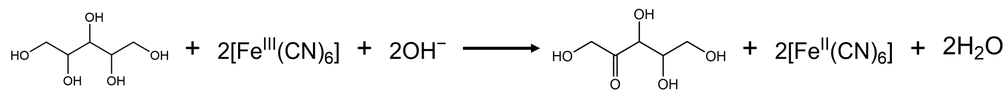
- The FTIR and Raman spectra reveal the formation of Fe–OH and Fe–O bonds in Fe(Xylitol), respectively, confirming the successful coordination between Fe and xylitol.



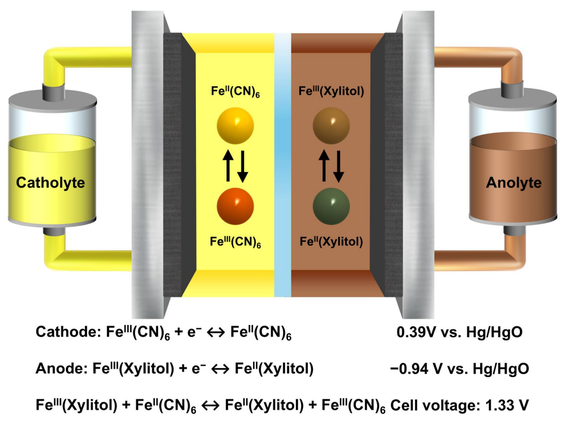
- Optimization of the OH− concentration revealed that 5 M KOH provides the best electrochemical performance for Fe(Xylitol).

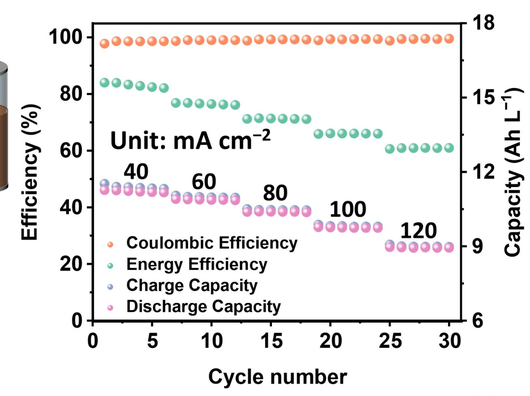


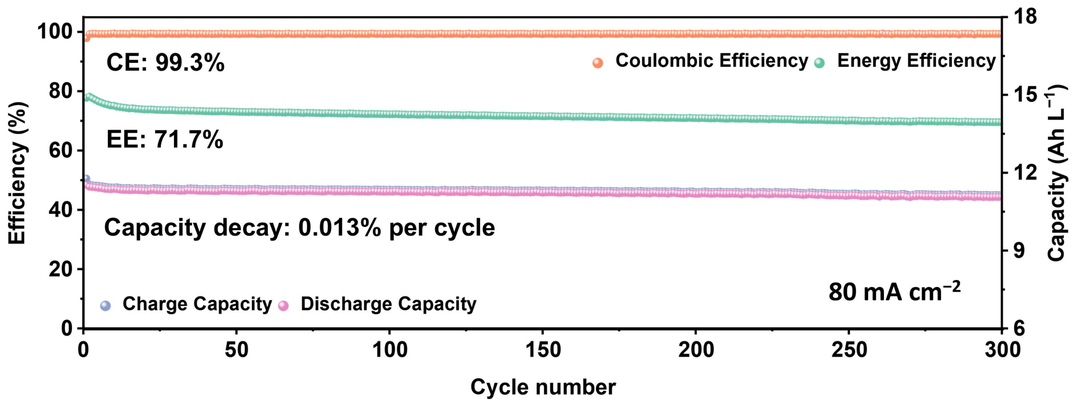
- Optimization of the Fe-to-xylitol ratio revealed that a 1:1 ratio provides the best electrochemical performance.



- Crossover of excess ligand to the Fe(CN)6 side reduces the stability of the FB by inducing self-discharge.







- The 0.5 M $Fe(CN)_6$ / 0.5 M Fe(Xylitol) FB single cell was operated at current densities from 40 to 120 mA cm^{-2}.
- Stable operation was achieved with >99% coulombic efficiency.
- At 80 mA cm^{-2}, the single cell operated for 300 cycles with an average energy efficiency of 71.7% and a capacity decay rate of 0.013% per cycle.

Conclusions

- Xylitol was proposed as a new ligand for iron-based complexes.
- The optimized electrolyte composition of 0.5 M Fe^{3+}, 0.5 M xylitol, and 5 M KOH exhibited stable electrochemical behavior.
- Fe(Xylitol) was demonstrated to be a promising anolyte candidate for flow batteries, as confirmed by single cell operation.
- These results highlight that nitrogen-free ligands can form stable iron complexes through effective chelation and be used as active materials for FBs.

Acknowledgment

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