Aqueous redox flow batteries using iron complex materials as redox couple

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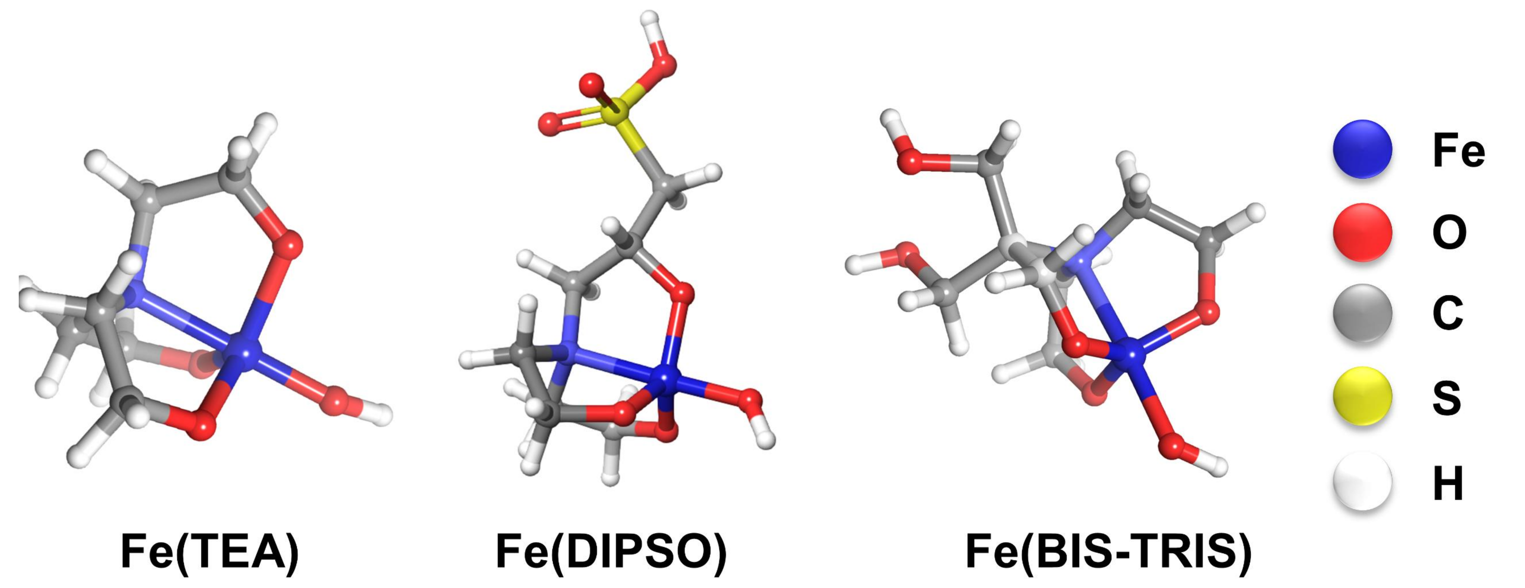
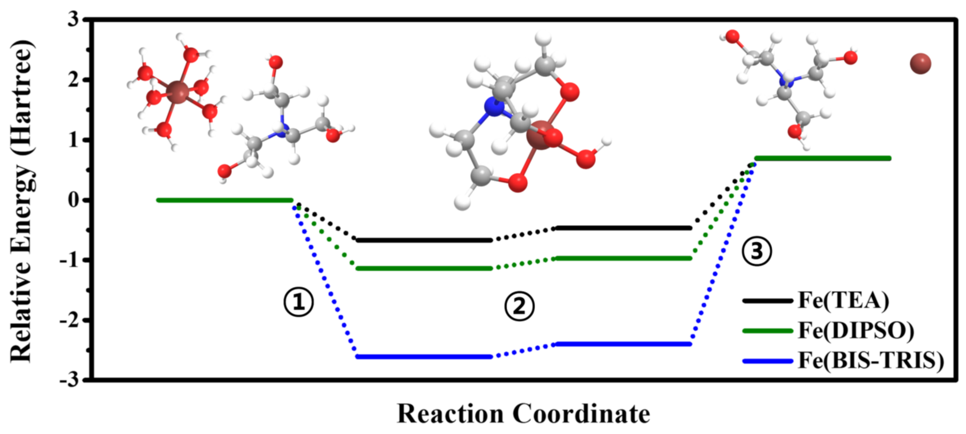
Introduction



- Iron-based active materials are ideal for RFBs due to their stable prices and the abundance of resources.
- The newly synthesized iron-organic complex, Fe(BIS-TRIS), has been introduced to address the stability, affordability, and performance limitations of RFBs that use existing iron-organic complexes.

Result and Discussion

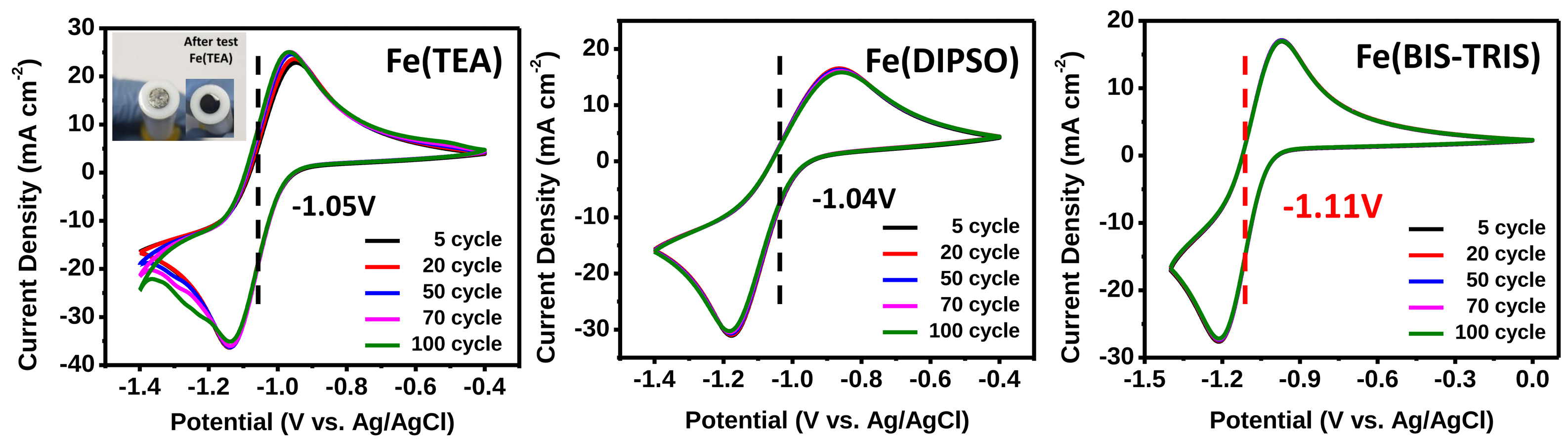


	HOMO (Hartree)	LUMO (Hartree)
Fe(TEA)	-0.817	-0.659
Fe(DIPSO)	-0.735	-0.661
Fe(BIS-TRIS)	-0.739	**-0.639**

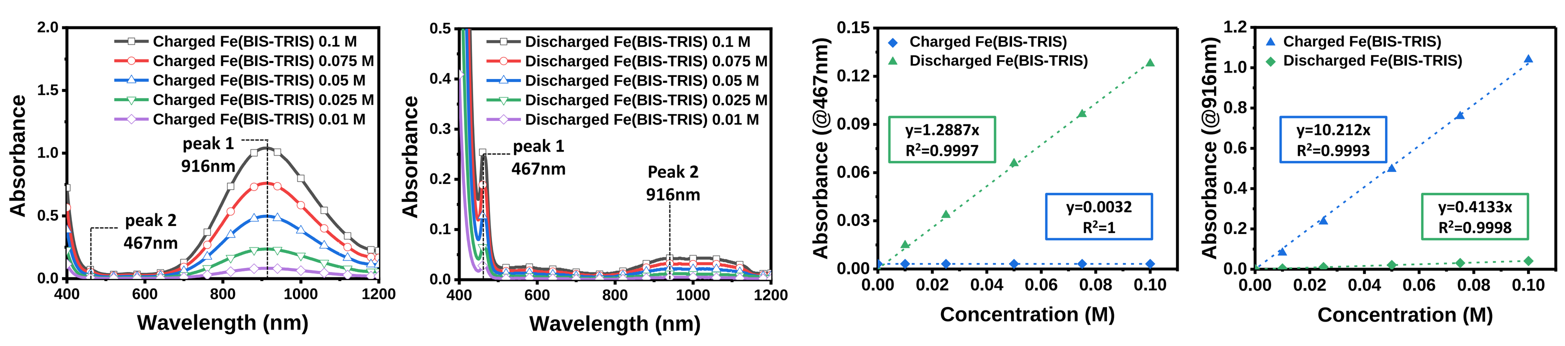
	Fe(DIPSO)		Fe(BIS-TRIS)	
	Fe	DIPSO	Fe	BIS-TRIS
Price of materials ($\$ g^{-1}$) 1)	0.069	1.877	0.069	0.430
	1.946		**0.499**	

1) The cost of chemicals was surveyed at webpages of Alfa Aesar at the largest volume in stock [https://www.alfa.co.kr/, last visited on 8th Jan. 2022]

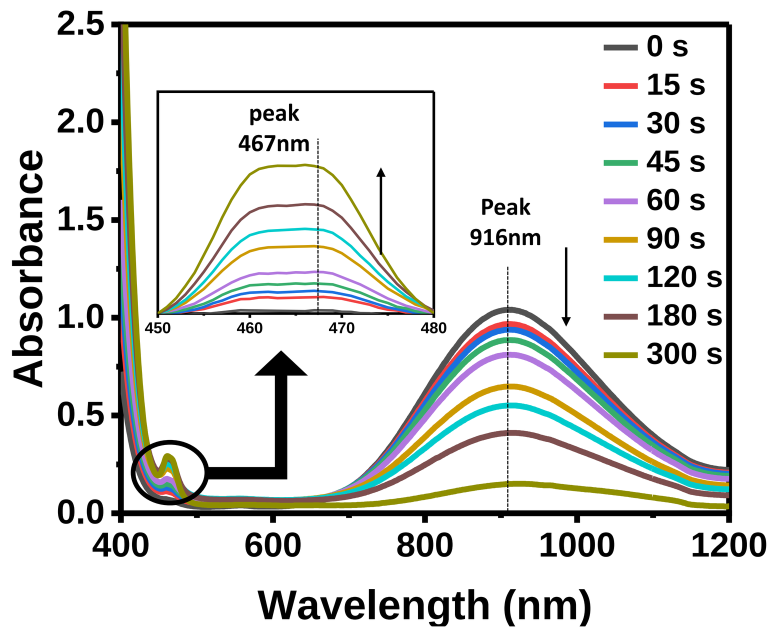
- DFT calculations affirm that Fe(BIS-TRIS) exhibits greater stability and lower redox potential than traditional materials, qualifying it as a promising anodic active material.
- Fe(BIS-TRIS) is more cost-effective than Fe(DIPSO), previously suggested as an alternative to Fe(TEA), suggesting that Fe(BIS-TRIS) offers advantages in stability, performance, and cost.



- Cyclic voltammetry (CV) tests verify that Fe(BIS-TRIS) possesses the most negative potential, facilitating its use as an anodic active material.
- CV testing over 100 cycles substantiates the stability of Fe(BIS-TRIS), contrasting with Fe(TEA), which is electrochemically unstable.



- A method for analyzing the state of charge (SOC) of electrolytes was established by examining charged and discharged Fe(BIS-TRIS) using UV-VIS spectroscopy.



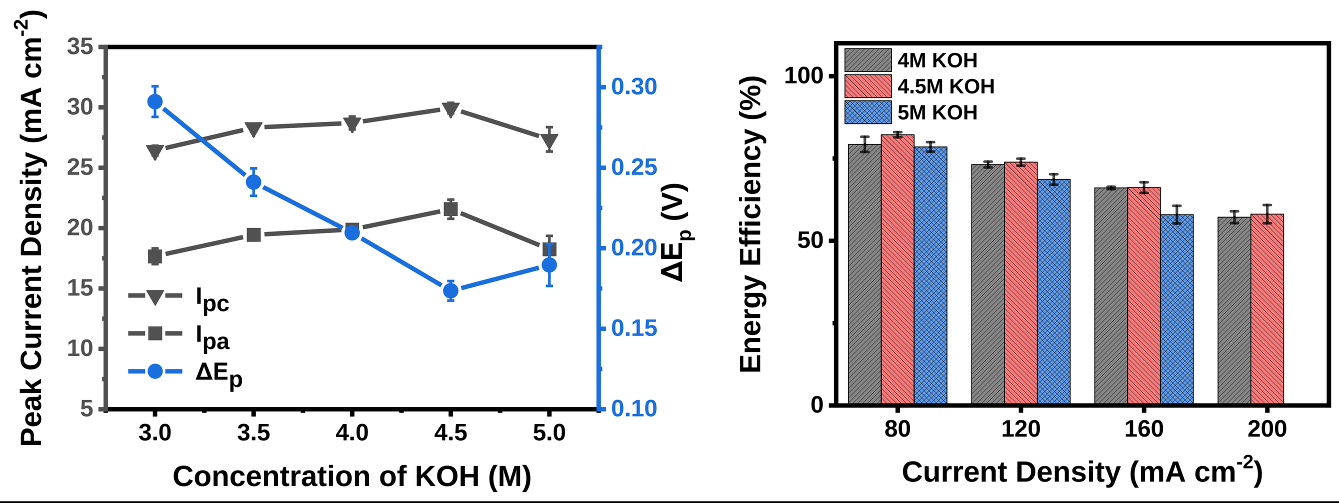
- Self-discharge can occur due to the reaction of oxygen with the charged Fe(BIS-TRIS) electrolyte.
- Self-discharging reactions

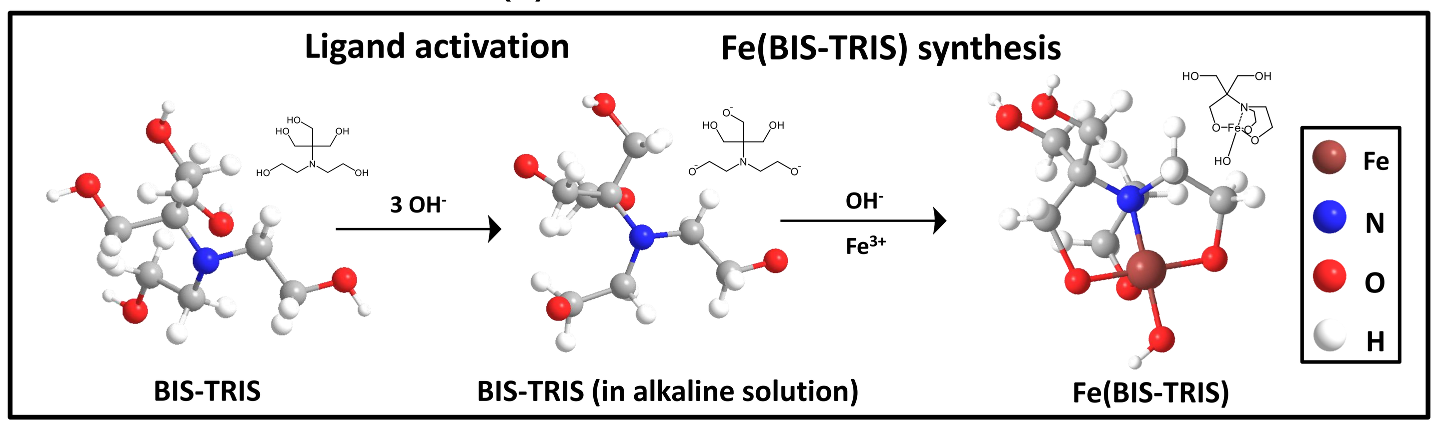
$O_2 + 2H_2O + 4e^- \rightarrow 4OH^-$

$Fe(II)(BIS\text{-}TRIS)^{2-} \rightarrow Fe(III)(BIS\text{-}TRIS)^- + e^-$

$\mathbf{O_2 + 4Fe(II)(BIS\text{-}TRIS)^{2-} + 2H_2O}$

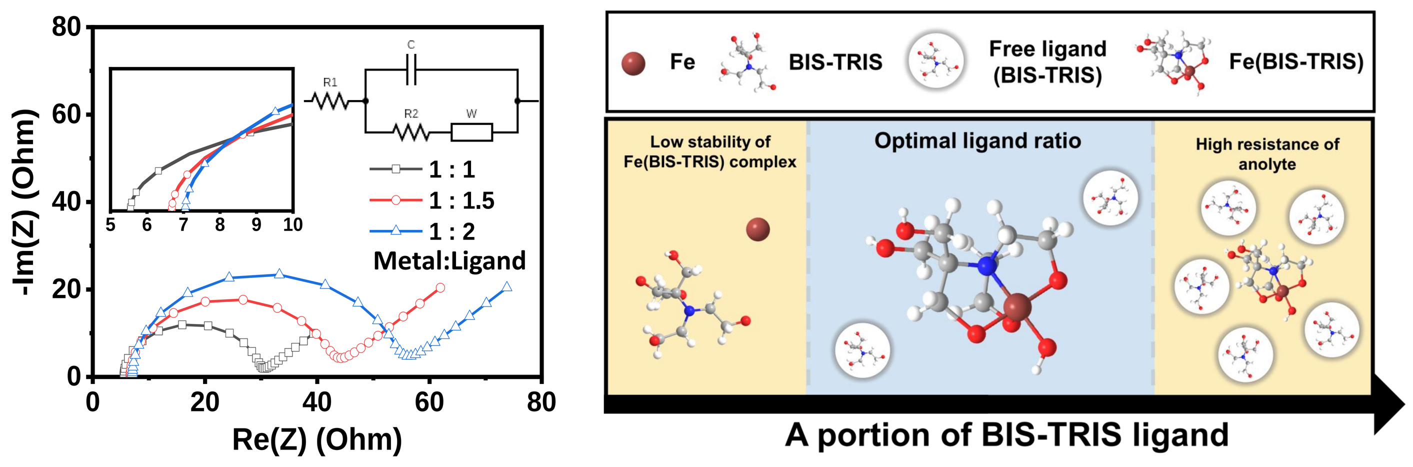
$\mathbf{\rightarrow 4\ Fe(III)(BIS\text{-}TRIS)^- + 4OH^-}$

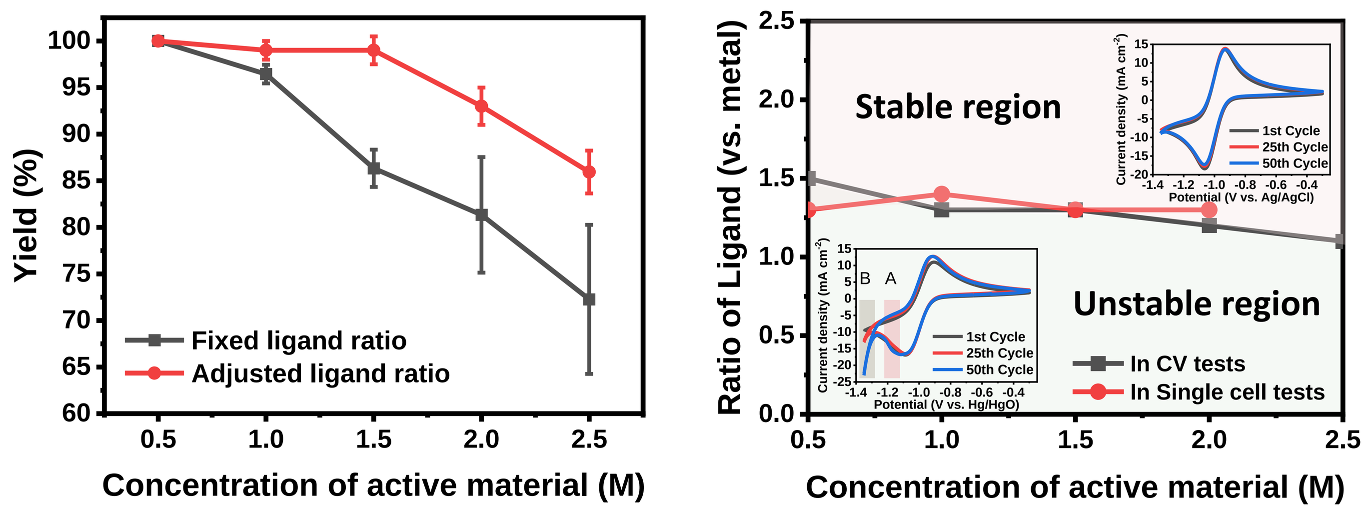




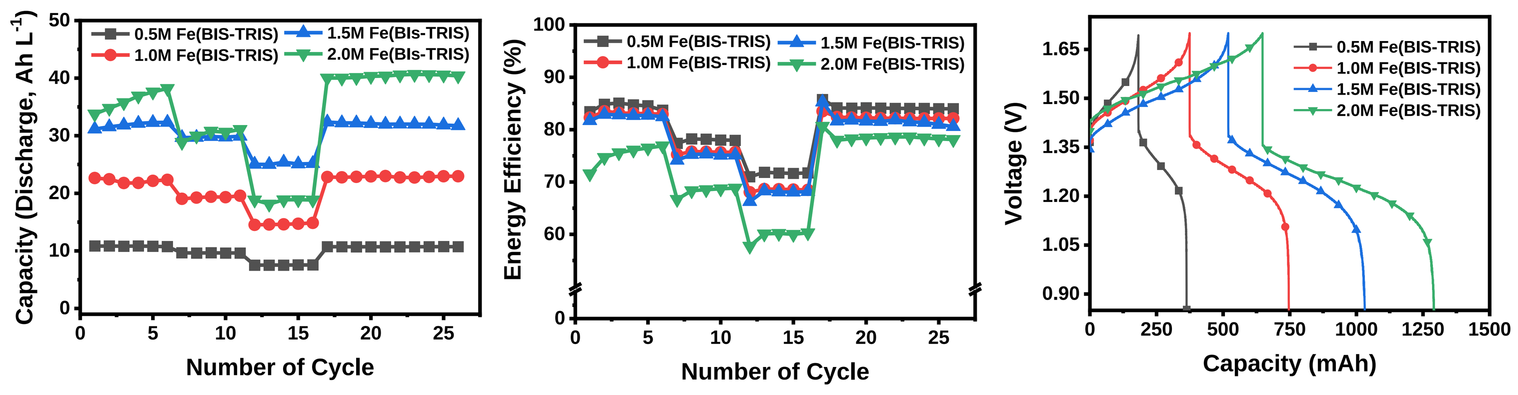
- The concentration of KOH, which acts as a ligand activator and supporting electrolyte, had been optimized.

(3 KOH / 1 Ligand + 1 KOH / 1 complex + 2.25M KOH for SE)



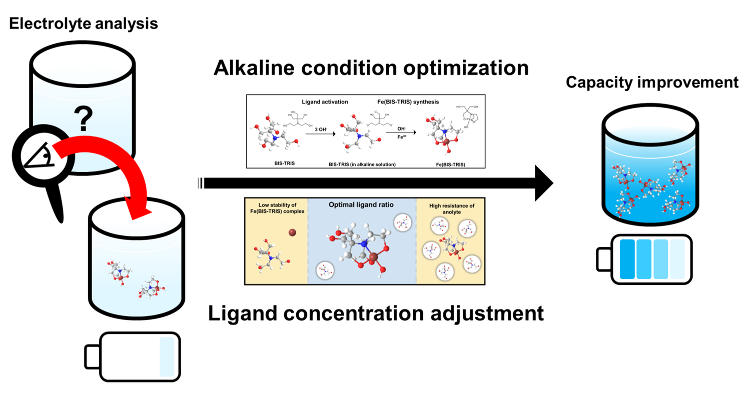


- A synthesis method and electrolyte optimization were carried out to enhance the solubility of the material.
- The optimal ligand concentration was determined, and the synthesis process was adjusted to decrease electrolyte viscosity and increase the yield of the active substance synthesis.



- Operating the RFB cell with the optimized electrolyte resulted in an increase in capacity from 12 Ah/L to 40.4 Ah/L.

Conclusion



- The newly synthesized Fe(BIS-TRIS) was stable and exhibited higher performance
- An optical method to confirm the state of charge has been established by analyzing the electrolyte, and its reactivity with oxygen has been confirmed.
- High solubility of the anodic active material was achieved through electrolyte optimization, and a capacity of 40.4 Ah/L was reached through actual cell operation.

Acknowledgment

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