Quantitative Investigation on Lithium Polysulfide Adsorption of MXene Compositions for High Performance Li-S Batteries

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Project Goal: Determining lithium polysulfide adsorption capacity of different MXene compositions

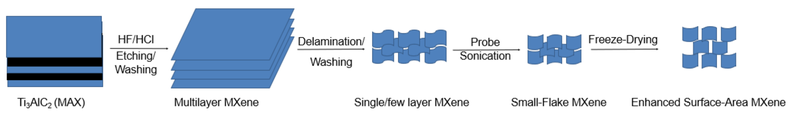
Introduction

- **Lithium-Sulfur batteries (LSBs)** have attracted a lot of attention because of their high theoretical energy density and relative abundance of their host materials
  - Challenges such as low conductivity of sulfur and dissolution of intermediate **lithium polysulfides** (LiPS) in the electrolyte hinders the practical utility of LSBs due to poor cycle life
- **MXenes** are a two-dimensional transition metal carbides and nitrides with high conductivity and rich surface functionalities, making them an appealing cathode host material for LSBs

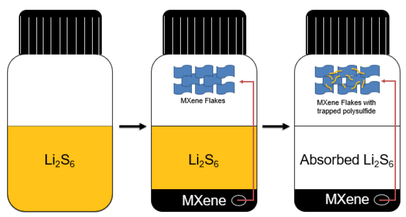
This study focuses on the quantification of MXene adsorption capacity of LiPSs

Experimental Section

MXENE SYNTHESIS



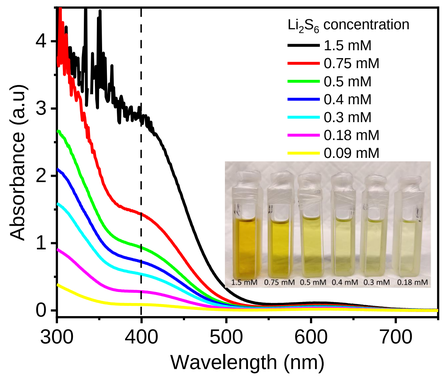
POLYSULFIDE ABSORPTION STUDIES

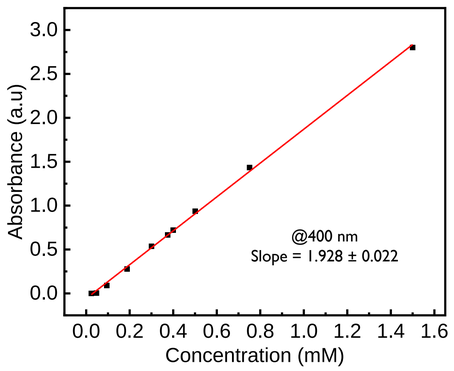


CHARACTERIZATION TECHNIQUES

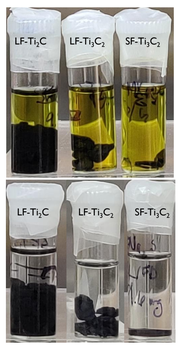
- Flake size was measured with dynamic light scattering (Zetasizer)
- UV-Vis spectrophotometer was used to determine the concentrations of supernatants before and after LiPS adsorption.
- Scanning electron microscopy (SEM) was used for imaging the surface topography and the composition (EDS elemental analysis).

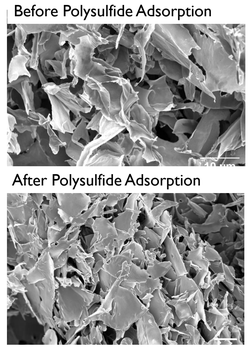
Data/Results

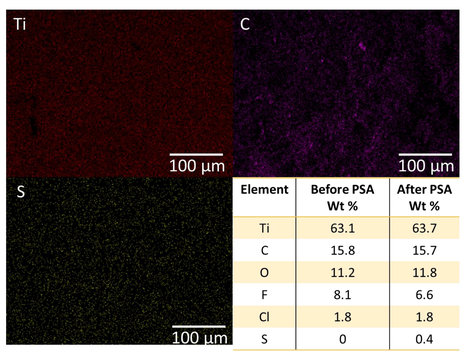




- Calibration curve made by collecting spectra of different concentrations of Li_2S_6, follows Beer-Lambert's law (A=εbC).

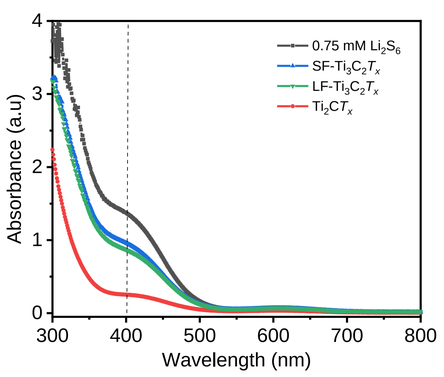


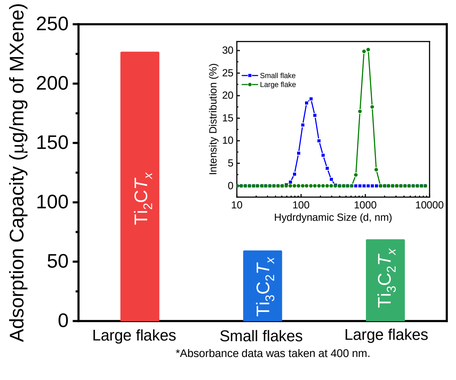




Element	Before PSA Wt %	After PSA Wt %
Ti	63.1	63.7
C	15.8	15.7
O	11.2	11.8
F	8.1	6.6
Cl	1.8	1.8
S	0	0.4

- The morphology of the MXene flakes remained the same after polysulfide adsorption
- The energy-dispersive X-ray spectroscopy (EDS) reveals the presence of sulfur uniformly throughout the MXene





*Absorbance data was taken at 400 nm.

- Ti_2C has the highest absorption capacity, far surpassing the other tested materials.

Conclusion

- **Lithium polysulfide adsorption** capacity is quantified using UV-Vis spectrophotometer
  - LF-$Ti_3C_2T_x$: ~68 mg of LiPS adsorbed/gram of MXene
  - SF-Ti_3CNT_x: ~58 mg of LiPS adsorbed/gram of MXene
  - Ti_2CT_x**:** ~226 mg of LiPS adsorbed/gram of MXene
  - Rich surface functionalities and high polarity are responsible for the trapping of polysulfides on MXene surface
  - More work has to be done to explain why Ti_2C has a higher adsorption capacity
- LiPSs uniform trapping on MXene surface was further confirmed by EDS elemental mapping analysis

This study provides the suitability of Ti-based MXenes as cathodes for long cycle life Li-S batteries.

Future Work

- Repeat the absorbance tests to verify current data
  - Error bars to be added for accurate quantification
- Expand the lithium polysulfide adsorption studies to other MXene compositions to screen the better polysulfide adsorbing MXene.
- Assembly of Li-S half cells with ideal MXene candidates as cathode material to evaluate their performance

References

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Acknowledgements

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