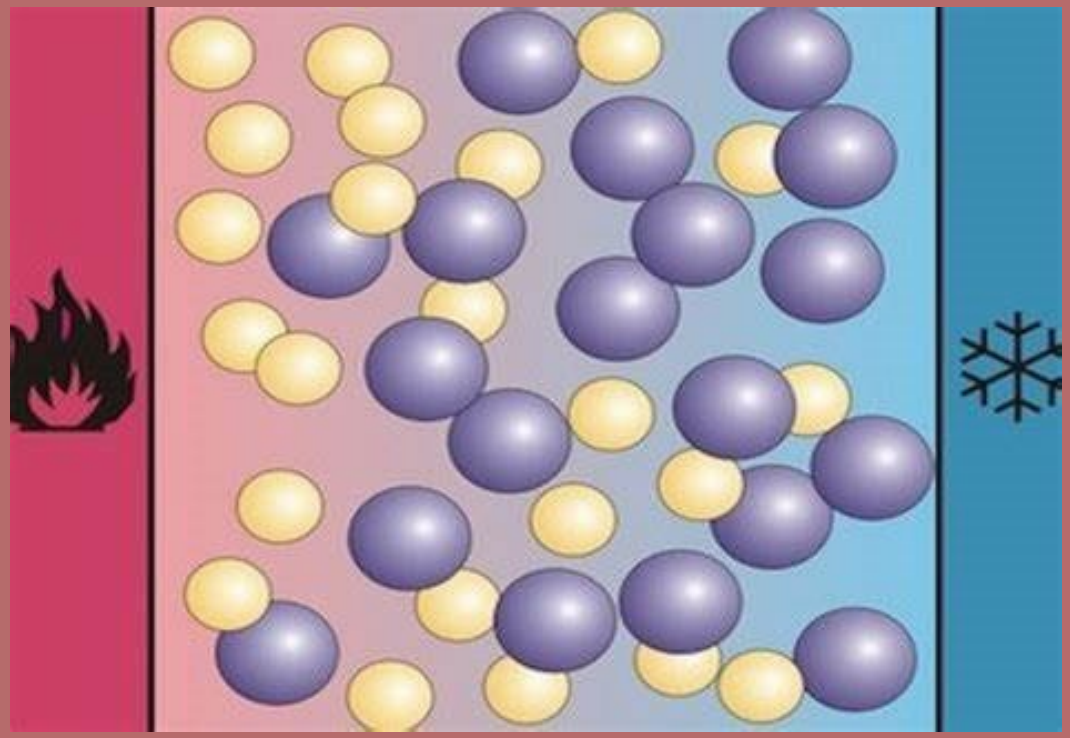
Analyzing the Soret Coefficient using time resolved FTIR-ATR Data

Ashley David, Dr. Daniel Hallinan

2022 President's Showcase

Steve Madden Undergraduate Research Award



Overview

01 Soret Effect

02 FTIR-ATR Technique

03 Methods

04 Results

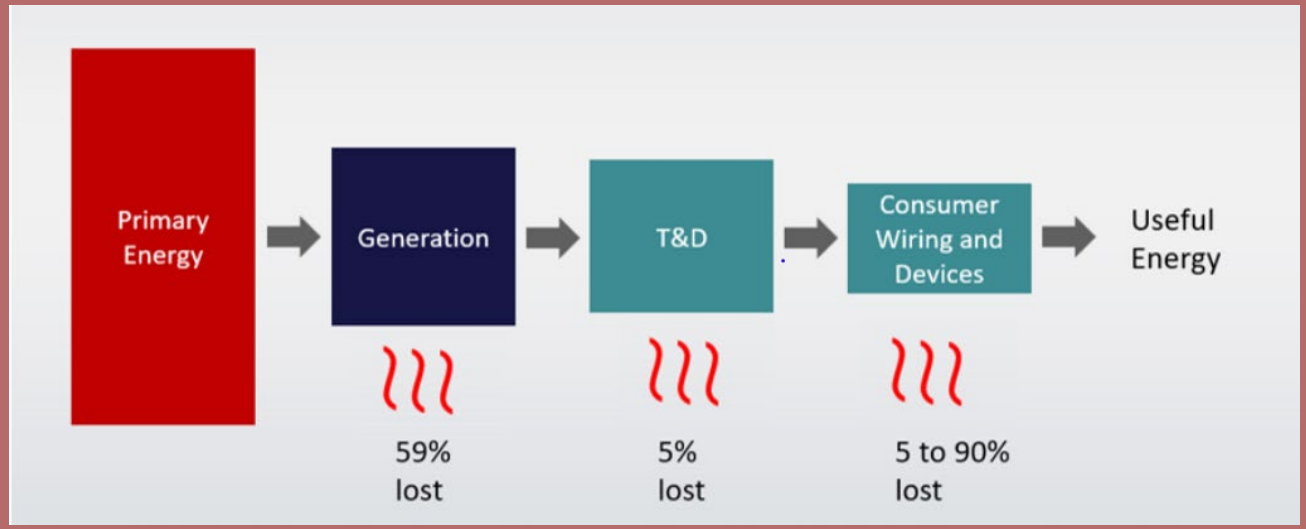
05 Future Work

01

How to decelerate Energy Consumption?

"66% of the primary energy used to create electricity is wasted by the time the electricity arrives at the customer meter."

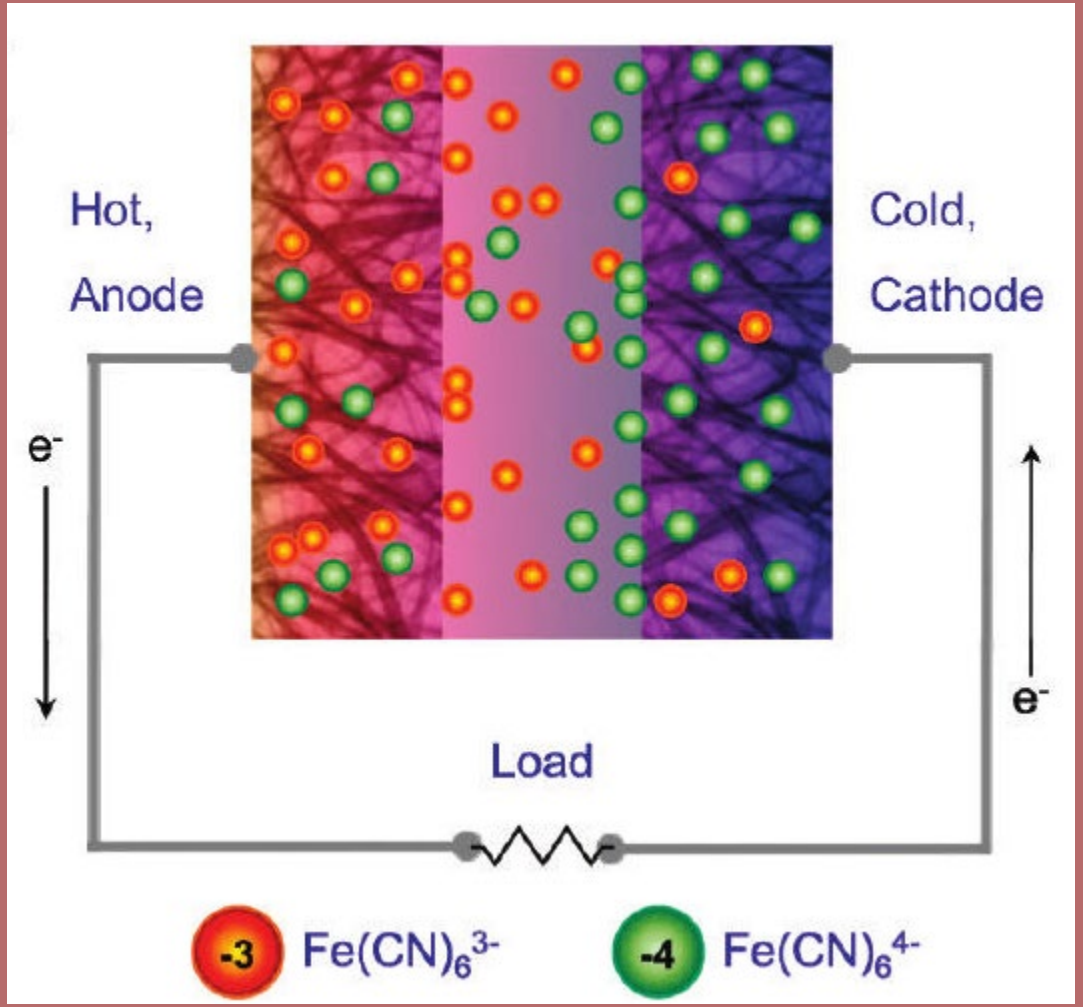
- Recapture waste heat
- Capital loss
- Land loss
- Fossil fuels



How Much Primary Energy Is Wasted Before Consumers See Value from Electricity? - Enerdynamics," www.enerdynamics.com. https://www.enerdynamics.com/Energy-Currents_Blog/How-Much-Primary-Energy-Is-Wasted-Before-Consumers-See-Value-from-Electricity.aspx

Soret Effect

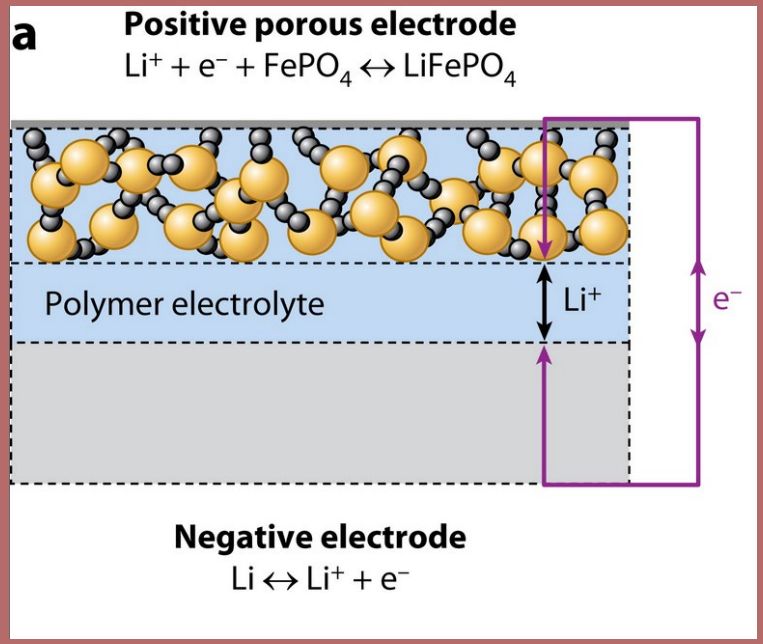
- Thermal Diffusion/Fickian Diffusion
- Steady state
- Application:
  - Solid state thermogalvanic cells

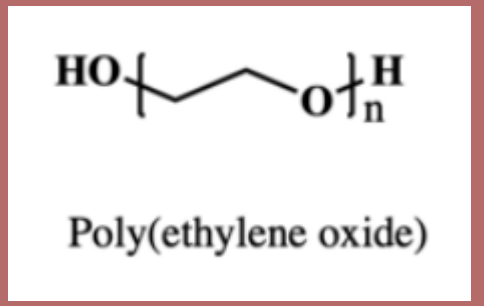


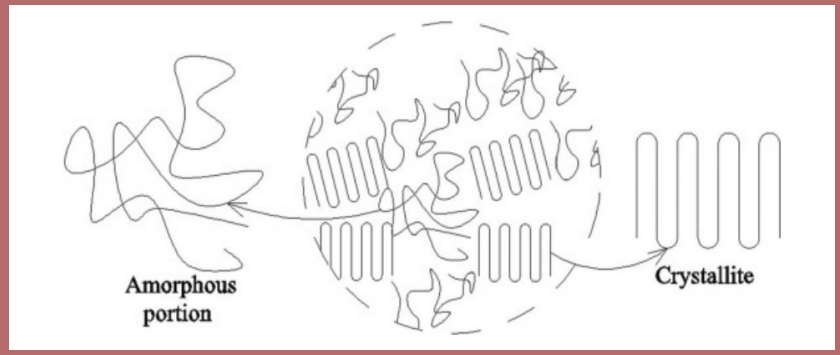
Renchong Hu, Baratunde A. Cola, Nanda Haram, Joseph N. Barisci, Sergey Lee, Stephanie Stoughton, Gordon Wallace, Chee Too, Michael Thomas, Adrian Gestos, Marilou E. dela Cruz, John P. Ferraris, Anvar A. Zakhidov and Ray H. Baughman (2010) Harvesting Waste Thermal Energy Using a Carbon-Nanotube-Based Thermo-Electrochemical Cell. *Nano Lett.*, Article ASAP doi: 10.1021/nl903267

PEO/LiTFSi

- Poly(ethylene oxide)– repeat units
- Polymer electrolyte
- Molecular design and cation transport
- Solid state electrolytes advantageous over liquid electrolytes



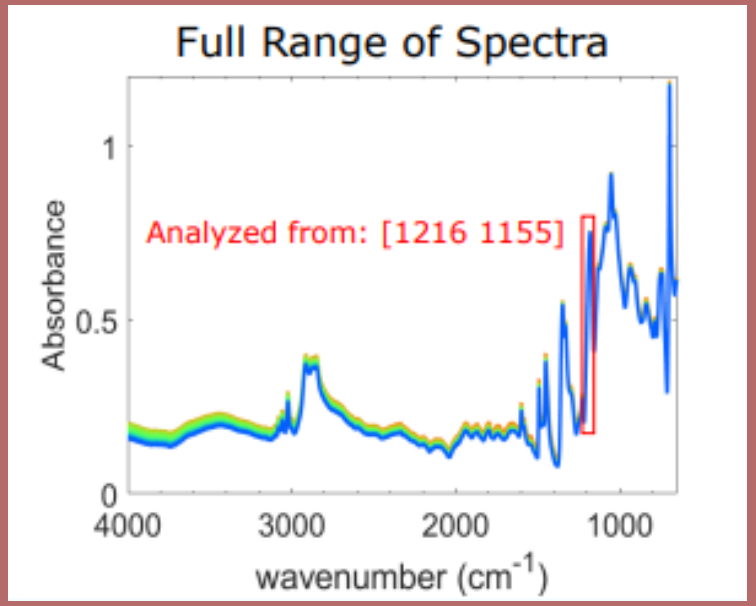




Hallinan, Daniel T.; Balsara, Nitash P. (2013-07-01). "Polymer Electrolytes". Annual Review of Materials Research. ***43*** (1): 503–525. Bibcode:2013AnRMS..43..503H. doi:10.1146/annurev-matsci-071312-121705. ISSN 1531-7331.

FTIR-ATR

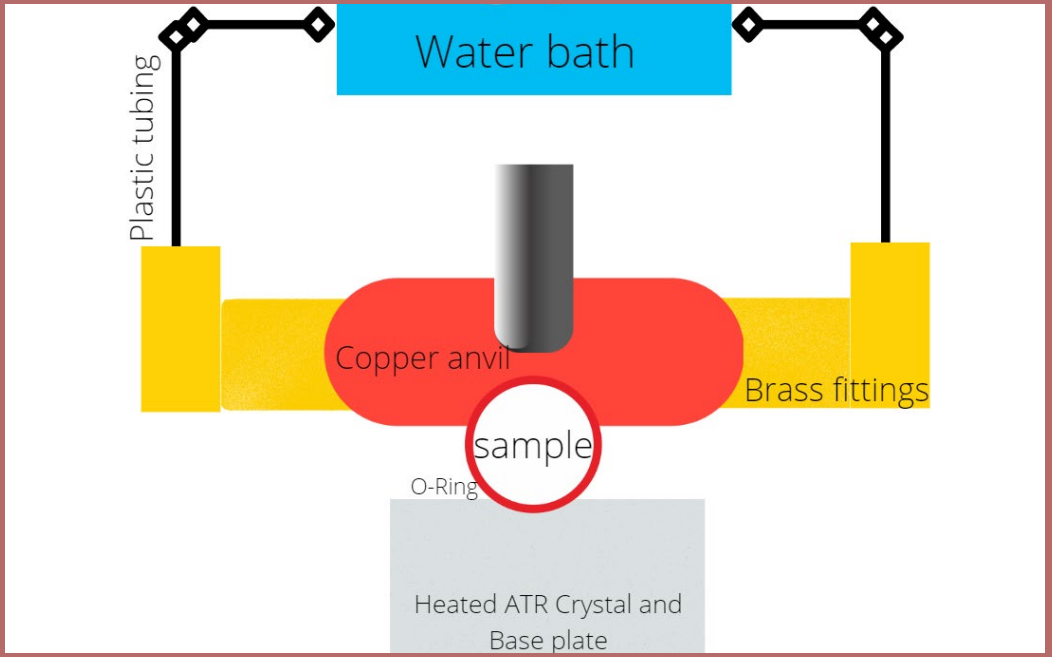
- Fourier transform infrared spectroscopy – attenuated total reflectance
- Novel method diffusion coefficient measurement developed from prior work[1]
- Infrared Absorbance
- Polymer Electrolyte Samples
- Beer lambert law
- Wave number: [1216 1155]



[1]Kim, K.; *Hallinan, D. T., Lithium Salt Diffusion in Diblock Copolymer Electrolyte Using Fourier Transform Infrared Spectroscopy. The Journal of Physical Chemistry B **2020**, 124 (10), 2040-2047, DOI: 10.1021/acs.jpcb.9b11446.

Methods: FTIR

- Heated Golden Gate ATR Accessory
- Custom copper anvil
- Initial Calibrations
- Mercury cadmium terlluride (MCT detector)
- Gradient induced, returned to isothermal state
- 6 hours



Water Bath Temp (°C)	Golden Gate Temp (°C)
65	75
62.5	77.5
60	80

Methods: Samples

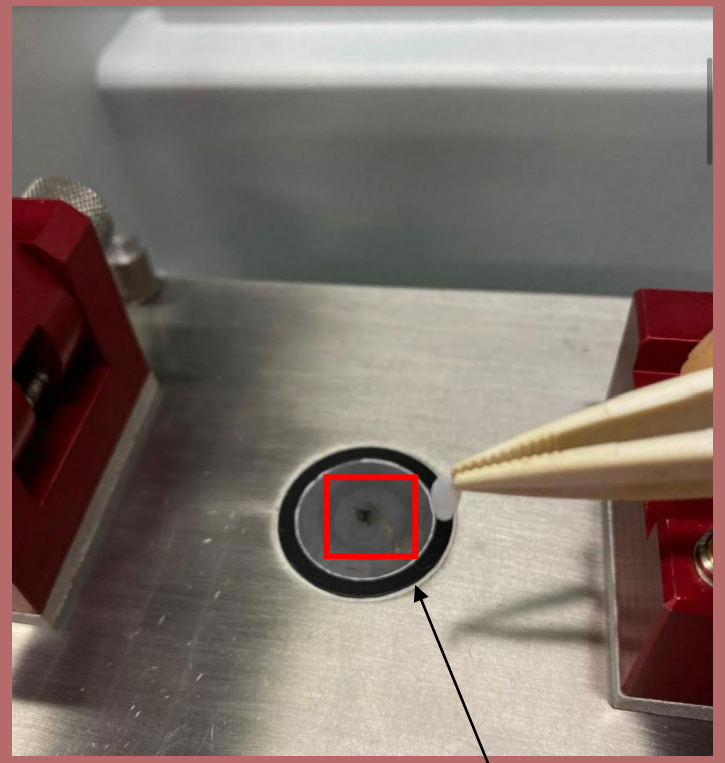
Sample Prep:

- Glovebox

- Polystyrene–b–poly(ethylene oxide)(SEO), and lithium bis-trifluoromethanesulfonylimide (LiTFSi)

- molar ratio: r=0.10 []

- Punched disks & pressed

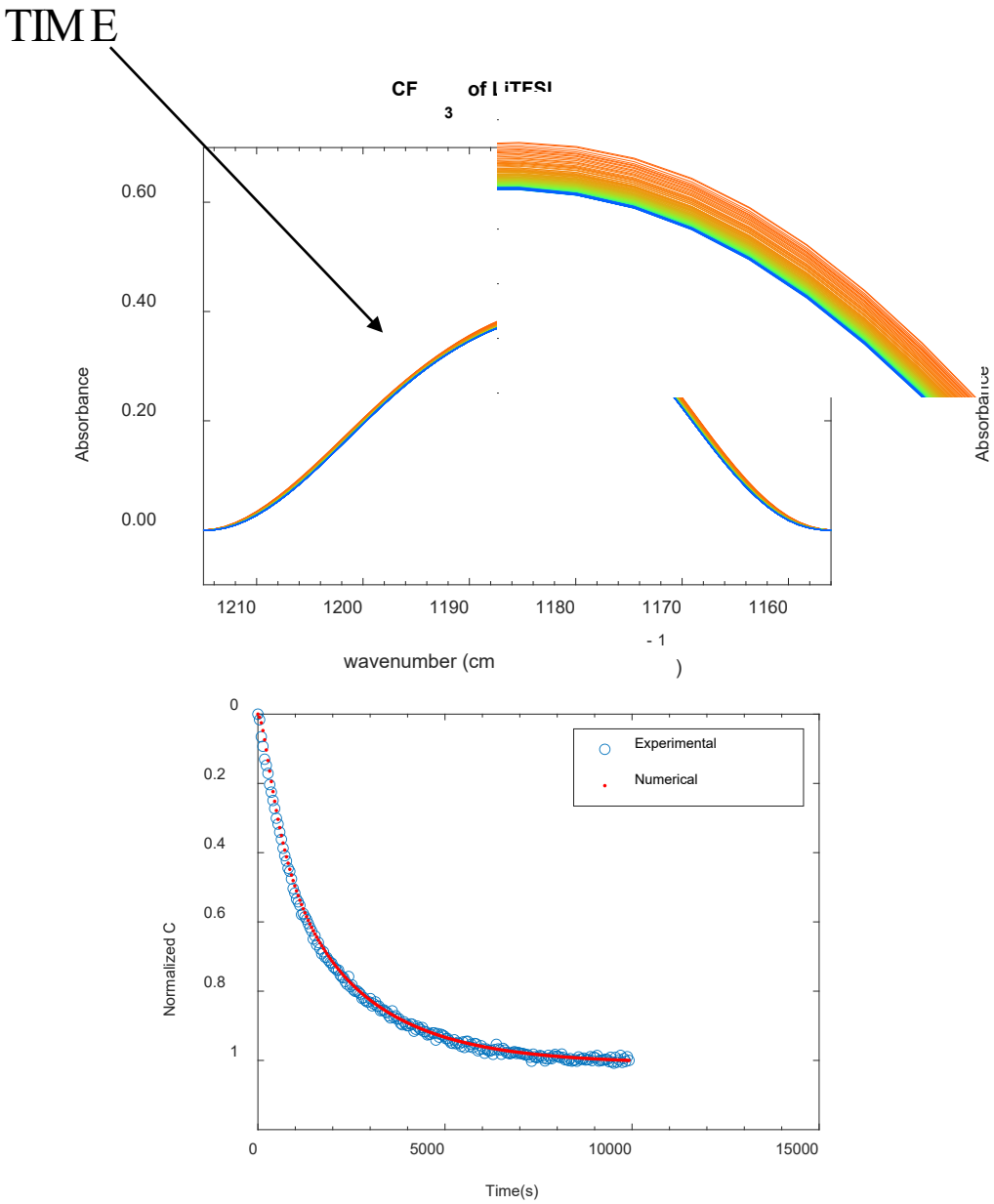


Concentration r=0.10	Thickness (mm)
1	0.103
2	0.283
3	0.294
4	0.302
5	0.273

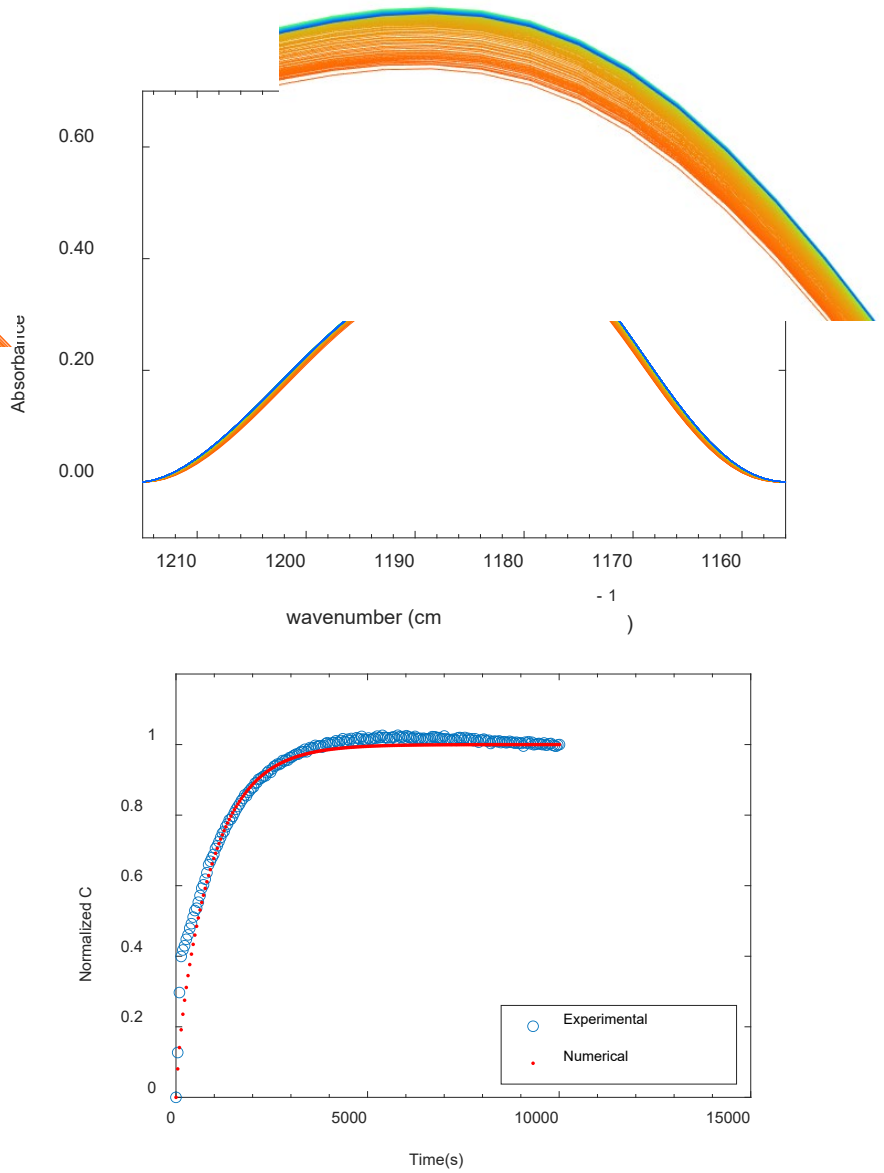
5 Step MATLAB Script:

Data transfer
conversion
integration
Numerical
Analytical

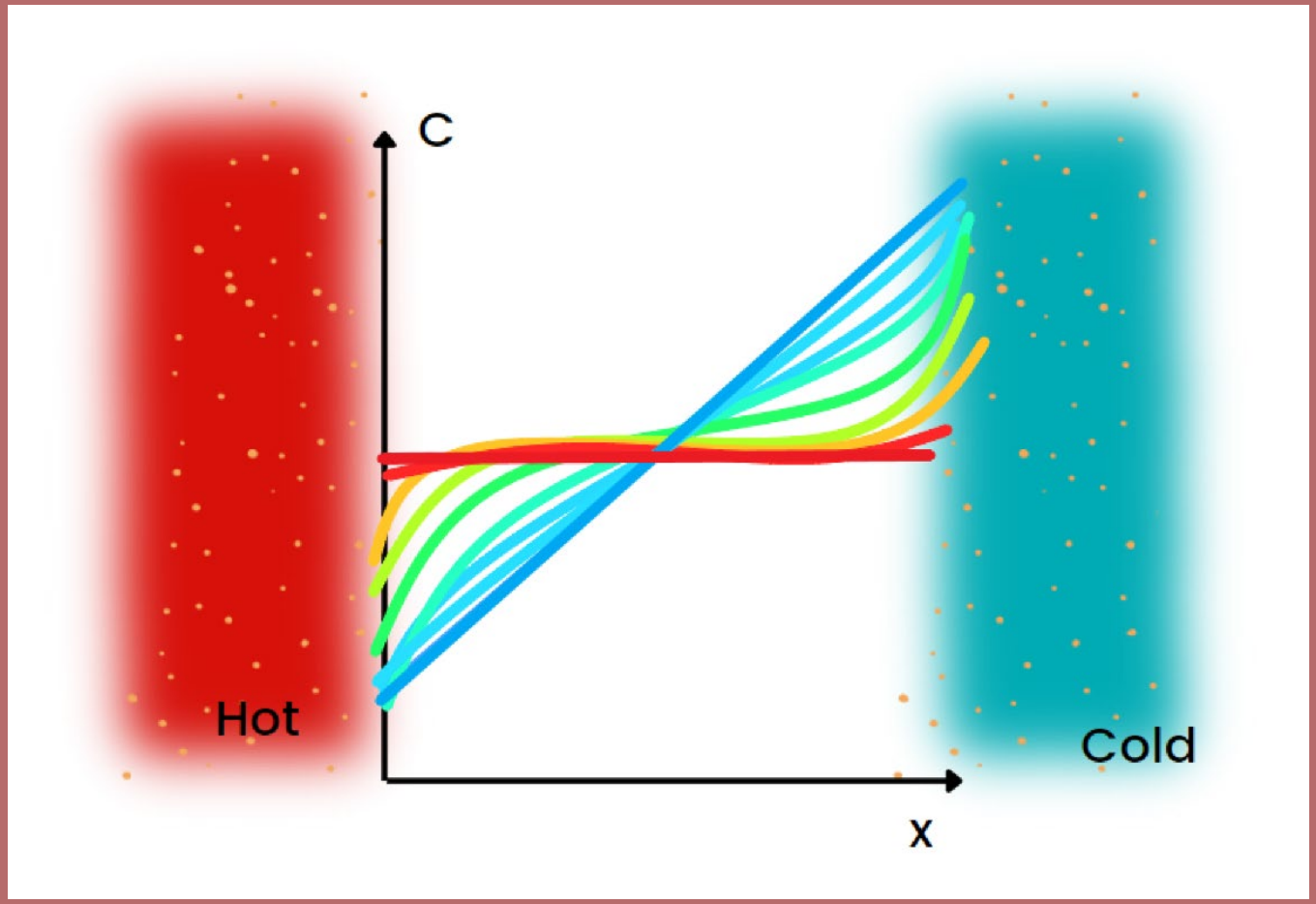
Thermal Diffusion (70/70→60/80)



Fickian Diffusion (60/80→ 70/70)



FTIR-ATR



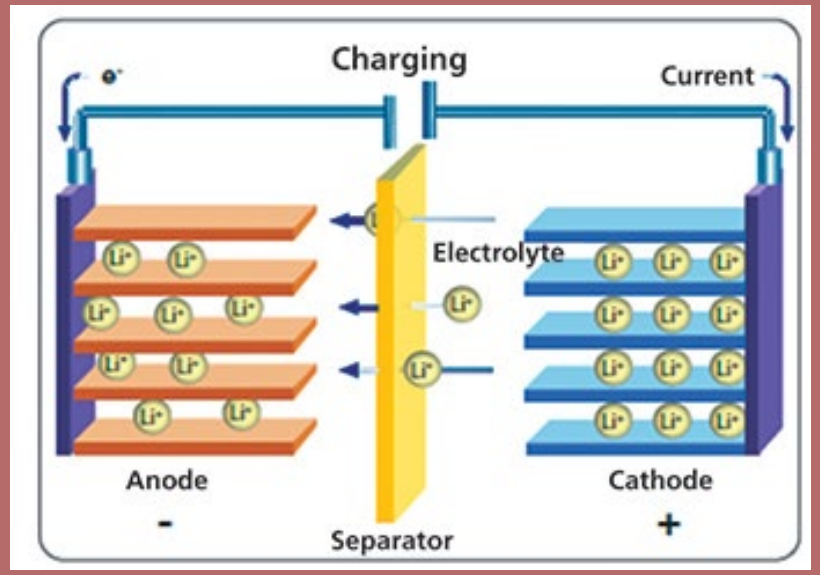
$$C(t)\ \alpha\ C(x)$$

Results: Fickian Diffusion

62.5/77.5→70/70			
Experiment Number	D ($\frac{cm^2}{sec}$)	Average	Standard Deviation
1	1.92E-08	5.47E-08	2.62E-08
3	4.00e-08		
4	7.99E-08		
5	7.99E-08		

60/80→70/70			
Experiment Number	D ($\frac{cm^2}{sec}$)	Average	Standard Deviation
1	1.52E-08	4.88E-08	2.39E-08
3	4.00e-08		
4	7.99E-08		
5	5.99E-08		

Future Work



Research:

- Thermal Diffusion MATLAB Code
- Backward time step
- Concentrations
- Molar masses

Presentations:

- ECS Conference
- AIChE National Student Conference
- Submitting to Journal: November

Chawla, N.; Bharti, N.; Singh, S. Recent Advances in Non-Flammable Electrolytes for Safer Lithium-Ion Batteries. Batteries 2019, 5, 19. [CrossRef]

Special Thanks

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NSF

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Steve Madden IDEA Grant Award

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Dr. Daniel Hallinan

FAMU-FSU College of Engineering

FAMU/FSU COE Machine Shop