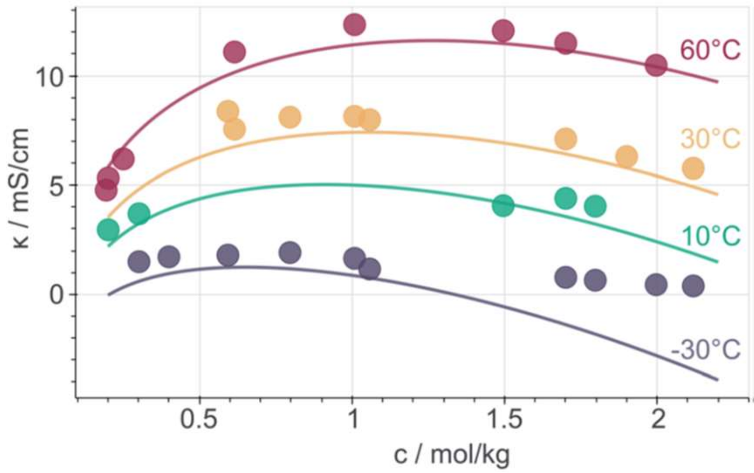
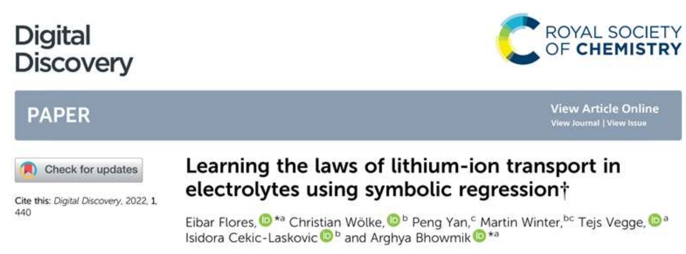
Prediction of low temperature electrolyte conductivity

Motivation

b. Fit on withheld set



- Authors modeled electrolyte conductivity as a function of
  - Li salt loading
  - Fraction of propylene carbonate in electrolyte
  - Temperature
- Basically conductivity = f(salt loading, PC fraction) at a given temperature
- Approach predicted good trends overall
  - Unable to capture the trends at low temperature



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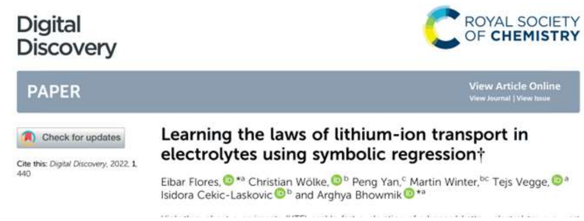
Eibar Flores,*[a] Christian Wölke,[b] Peng Yan,[c] Martin Winter,[bc] Tejs Vegge,[a] Isidora Cekic-Laskovic[b] and Arghya Bhowmik*[a]

Possible explanation for trends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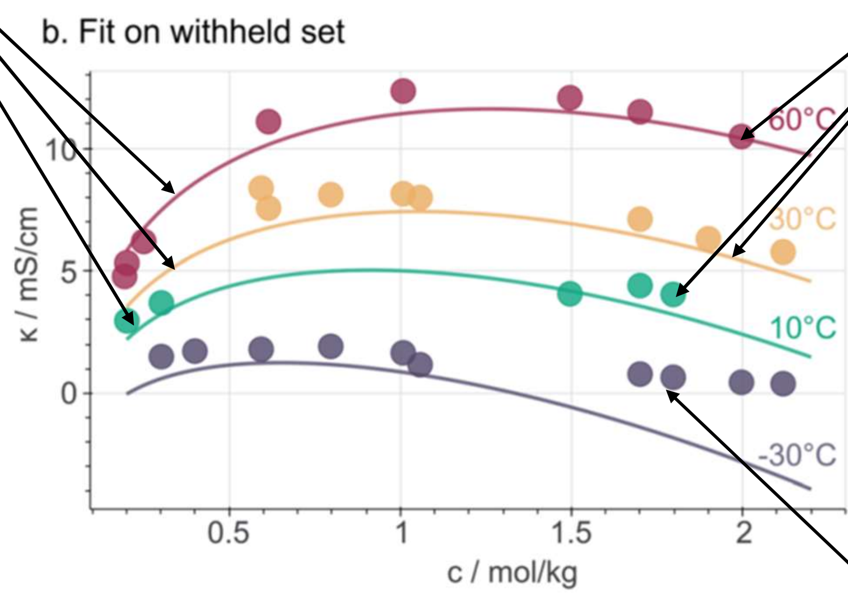
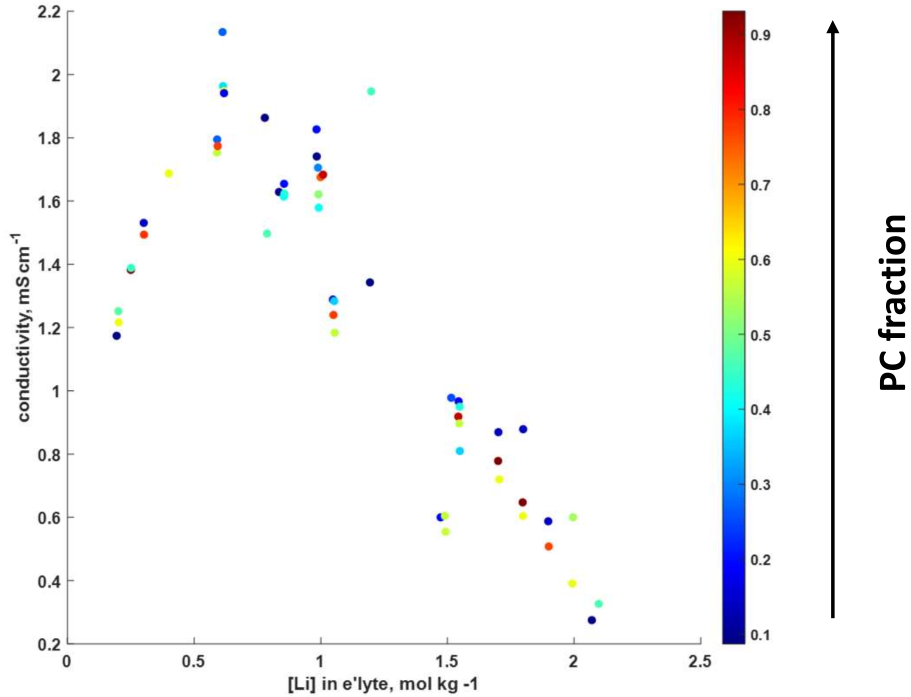
Increase with concentration i.e. “billiards” approximation

Falls due to ionic association



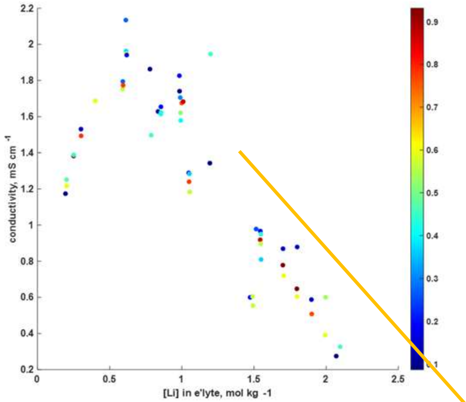
Ionic association ~ coagulation -> falls with lower temperature

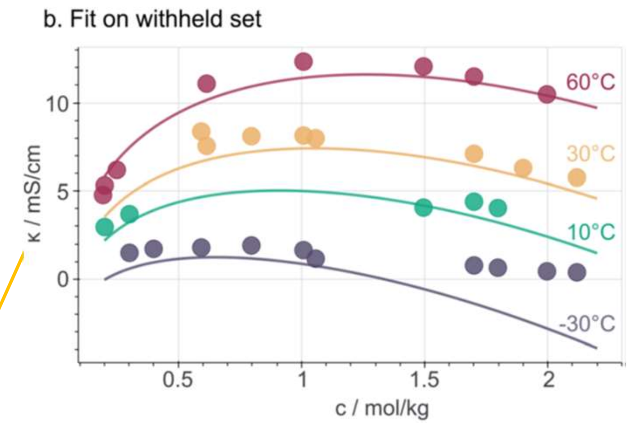
How does conductivity vary with salt loading and PC fraction at 243K?



- Zoomed in on the conductivity scale
  - Clearly defined trend with Li salt loading
  - Haphazard behaviour with PC fraction

Proposed corrections

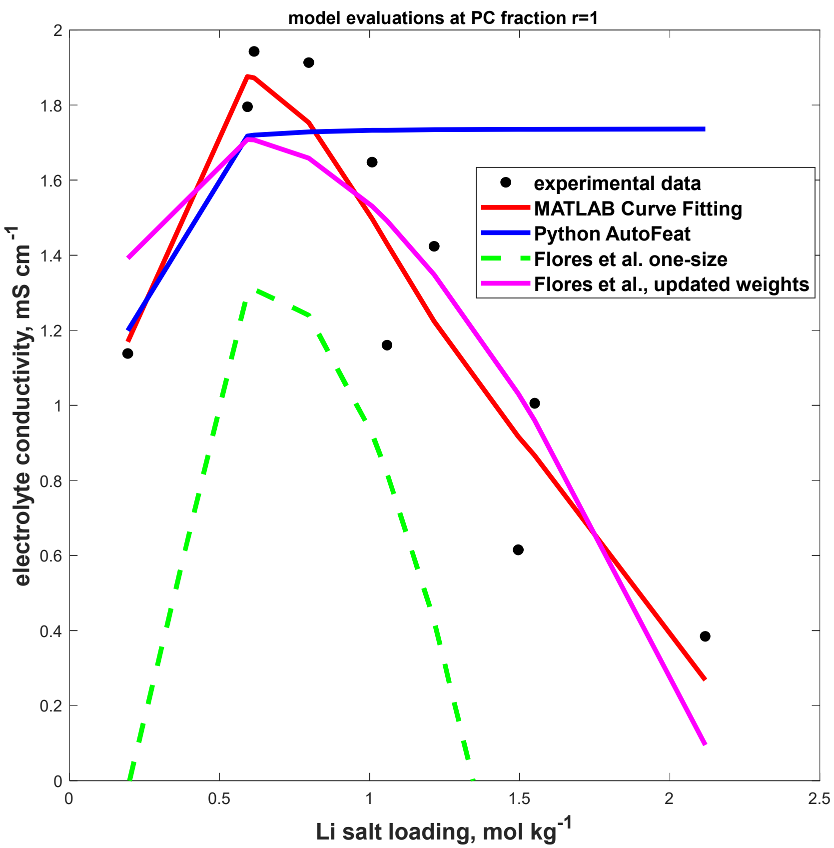




Method	Rationale	Package	Name
Fit a high (≥2)degree polynomial in c, force through zero	Behaviour at constant temperature is essentially dependent on c and not r	MATLAB Curve Fitting Toolbox	polynomial fitting
Train a symbolic regression model in the lower temperature regime	Possible need to change weights due to shallow trends at higher concentration	Python Autofeat	symbolic regression, low T
Use features from Flores et al but update weights in a linear combination, force through zero		Python ski-kitlearn	updated weights

- *c* = lithium salt loading, mol kg-1
- *r* = fraction of propylene carbonate in electrolyte solvent (along with ethylene carbonate and ethyl methyl carbonate)
- *T* = temperature (constant for this study)

Comparing different approaches

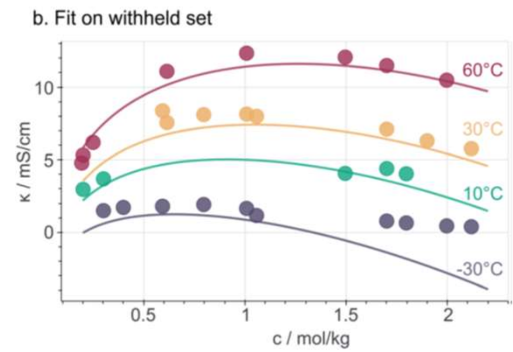


How do the fitted coefficients change?

$$\kappa = \beta_1 c + \cancel{\beta_2 T} + \beta_3 r^{\frac{1}{2}} c^{\frac{5}{2}} + \beta_4 T^2 c^{\frac{1}{4}}$$

Not implemented since we're considering constant temperature

Coefficient	Flores et al	Current effort
β_1	-5.11	-2.804
β_2	-0.04	0
β_3	-0.35	-0.059
β_4	2.73×10^{-4}	7.437×10^{-5}



- The higher value of β_1 moves the curve upwards
- Lower values for β_3 and β_4 help "shallow" the curve