

EILERS GRADUATE STUDENT FELLOWSHIP FINAL REPORT

EILERS FELLOW:	Shelby Brantley
FACULTY ADVISOR:	Dr. Steven Corcelli
REPORT PERIOD:	January - December 2020
PROJECT TITLE:	Understanding the Dynamics of Solid-Electrolyte Interphase in Sodium Ion Batteries with Fluoroethylene Additive
CONNECTION TO ND ENERGY'S RESEARCH AREAS (CHECK ALL THAT APPLY):	<input checked="" type="checkbox"/> Energy Conversion and Efficiency <input type="checkbox"/> Sustainable and Secure Nuclear <input checked="" type="checkbox"/> Smart Storage and Distribution <input type="checkbox"/> Transformation Solar <input type="checkbox"/> Sustainable Bio/Fossil Fuels <input type="checkbox"/> Transformative Wind

MAJOR GOALS AND ACCOMPLISHMENTS:

List your major research goals and provide a brief description of your accomplishments (1-2 sentences). Indicate the percentage completed for each goal. Please use a separate sheet to share additional details, technical results, charts, and graphics.

MAJOR RESEARCH GOALS	ACTUAL PERFORMANCE AND ACCOMPLISHMENTS	% OF GOAL COMPLETED
Identify the Components of the Electrolyte Solution Affected by the Additive	I determined that fluoroethylene carbonate has stronger interactions with itself than it does with any other electrolyte solution. Structurally, only ethylene carbonate is altered by the presence of fluoroethylene carbonate.	100%
Solvent Cage Analysis of the Methyl Thiocyanate Probe	The solvent cage has been identified surrounding the methyl thiocyanate probe and it has been determined that the cylindrical distribution functions sufficiently capture the solvent cage. Cylindrical distribution functions show that only ethylene carbonate is affected by the addition of fluoroethylene carbonate.	90%
Determine the Effects of Sodium on the Electrolyte Solution and Additive Mixtures	Sodium ion simulations were unable to be performed due to extended experimental timelines and the need to extend the current simulations further for better statistical averaging.	0%

RESEARCH OUTPUT:

Please provide detailed information below regarding any output resulting from your research project.

CATEGORY	INFORMATION
EXTERNAL PROPOSALS	(Sponsor, Project Title, PIs, Submission Date, Proposal Amount)
EXTERNAL AWARDS	(Sponsor, Project Title, PIs, Award Date, Award Amount)
JOURNAL ARTICLES	(Journal Name, Title, Authors, Submission Date, Publication Date, Volume #, Page #s)
BOOKS AND CHAPTERS	(Book Title, Chapter Title, Authors, Submission Date, Publication Date, Volume #, Page #s)
PUBLIC PRESENTATIONS, SEMINARS, LECTURES	(Event, Presentation Title, Presentation Date, Location)
AWARDS, PRIZES, RECOGNITIONS	(Purpose, Title, Date Received)
INTERNAL COLLABORATIONS FOSTERED	(Collaborator Name, Organization, Purpose of Affiliation)

EXTERNAL COLLABORATIONS FOSTERED	(Collaborator Name, Organization, Purpose of Affiliation) Dr. Amber Krummel, Colorado State University, Performing the experimental measurements on the electrolyte solutions
WEBSITE(S) FEATURING RESEARCH PROJECT	(URL)
OTHER PRODUCTS AND SERVICES (e.g., media reports, databases, software, models, curricula, instruments, education programs, outreach for ND Energy and other groups)	(Please describe each item in detail)

MAJOR GOALS AND ACCOMPLISHMENTS
(Additional Details, Technical Results, Charts and Graphics)

Rotational correlation functions provide information about which components have altered dynamics caused by the addition of FEC. The rotational correlation functions for the carbonyl bond of each electrolyte component can be seen in Figure 1. Visually, it is apparent that the only component with a significant dynamic change is FEC. The pure FEC solution shows much slower dynamics than the FEC molecules in the 1:1:1 DMC:DEC:EC with 5% FEC, revealing that when FEC is used as an additive with electrolyte solutions, it is able to move more dynamically. This suggests that the interactions between FEC and DMC, DEC, and EC are weaker than FEC-FEC interactions. Visually, DMC, DEC, and EC show no major changes in their dynamics, indicating their interaction strength is essentially unchanged by the addition of FEC. This provides evidence the differing properties of the solid-electrolyte interface (SEI) formed by electrolyte solutions with the FEC additive can be attributed to the dynamics of the FEC component.

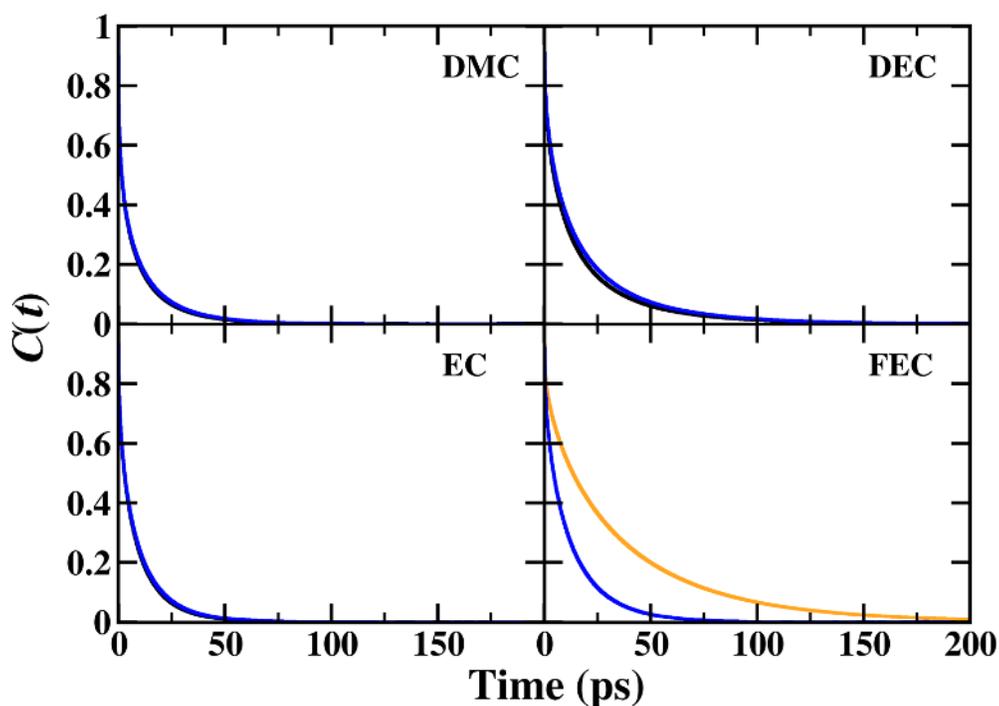


Figure 1: The rotational correlation functions calculated for the specified components of the pure FEC (gold), 1:1:1 DMC:DEC:EC (black), and 1:1:1 DMC:DEC:EC with 5% FEC by volume (blue) electrolyte solutions.

CDFs can also be calculated to evaluate the solvent environment surrounding the probe. These distributions provide a look at the different solvation shells for the individual solvent molecules, which provide information about where the molecule is interacting with the probe. CDFs are calculated in a similar manner to the RDFs, where the N of MeSCN is the reference atom and the carbonyl carbon is used for the density of DMC, DEC, and EC. The fluorinated carbon is used for the density of FEC. Resulting CDFs can be seen for 1:1:1 DMC:DEC:EC and 1:1:1 DMC:DEC:EC with 5% FEC by volume in Figures 2 and 3, respectively. Based on the rotational correlation functions, it is assumed that none of the components should show any structural changes. Surprisingly, EC has a much different CDF in 1:1:1 DMC:DEC:EC than when FEC is added to the solution. DMC and DEC remain essentially unaffected by the addition of FEC. This means when FEC is added to the electrolyte solution, FEC experiences changed interaction strengths as compared to the pure FEC solution, while EC experiences altered structural properties.

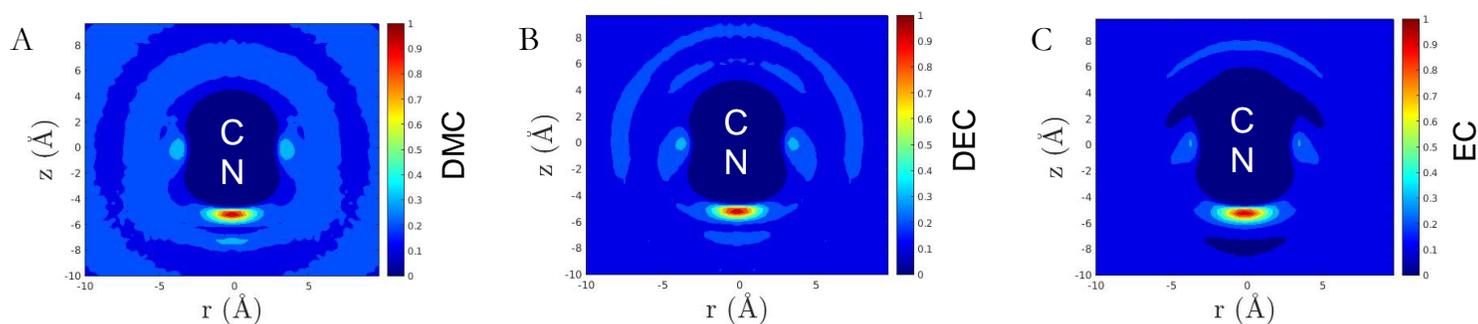


Figure 5.7: The cylindrical distribution functions for (A) DMC, (B) DEC, and (C) EC in the 1:1:1 DMC:DEC:EC mixture . All frequencies are normalized.

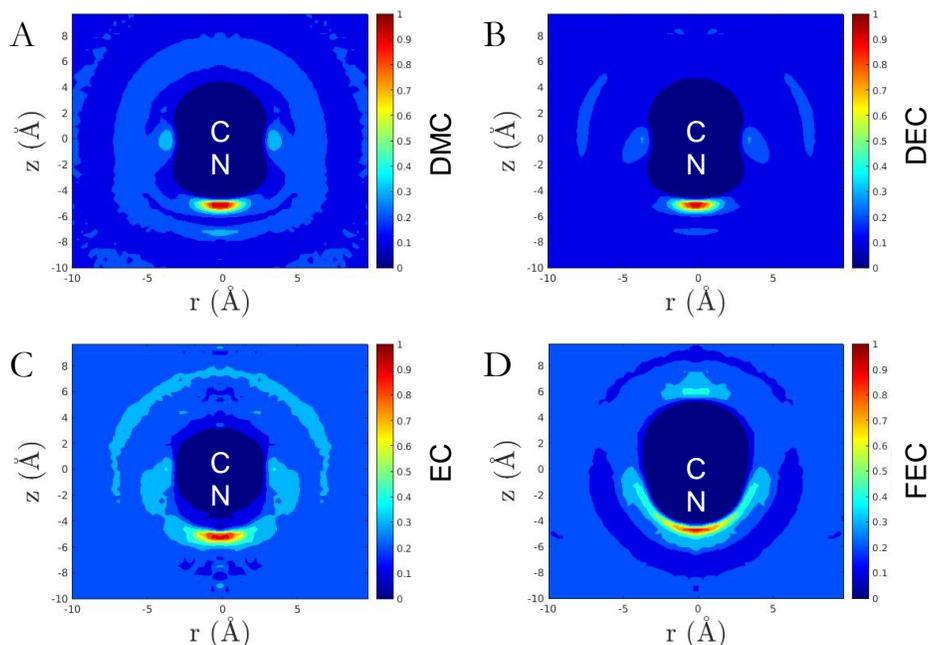


Figure 3: The cylindrical distribution functions for (A) DMC, (B) DEC, (C) EC, and (D) FEC for the 1:1:1 DMC:DEC:EC with 5% FEC by volume mixture. All frequencies are normalized.