

Abstract Submitted  
for the MAR17 Meeting of  
The American Physical Society

**Atomistic Structure and Dynamics of the Solvation Shell Formed by Organic Carbonates around Lithium Ions via Infrared Spectroscopies**  
DANIEL KURODA, KRISTEN FUFLE, Louisiana State University — Lithium-ion batteries have become ubiquitous to the portable energy storage industry, but efficiency issues still remain. Currently, most technological and scientific efforts are focused on the electrodes with little attention on the electrolyte. For example, simple fundamental questions about the lithium ion solvation shell composition in commercially used electrolytes have not been answered. Using a combination of linear and non-linear IR spectroscopies and theoretical calculations, we have carried out a thorough investigation of the solvation structure and dynamics of the lithium ion in various linear and cyclic carbonates at common battery electrolyte concentrations. Our studies show that carbonates coordinate the lithium ion tetrahedrally. They also reveal that linear and cyclic carbonates have contrasting dynamics in which cyclic carbonates present the most ordered structure. Finally, our experiments demonstrate that simple structural modifications in the linear carbonates impact significantly the microscopic interactions of the system. The stark differences in the solvation structure and dynamics among different carbonates reveal previously unknown details about the molecular level picture of these systems.

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Date submitted: 11 Nov 2016

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