Abstract Submitted
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The effect of co-solvent addition on Li-solvation in solvate electrolytes in Li-S batteries[1] KAH CHUN LAU, California State University Northridge, KIMBERLY A SEE, HENG-LIANG WU, MINJEONG SHIN, University of Illinois at Urbana-Champaign, LARRY A CURTISS, Argonne National Laboratory, ANDREW A GEWIRTH, University of Illinois at Urbana-Champaign — Li?S batteries are a promising next-generation battery technology. Due to the formation of soluble polysulfides during cell operation, the electrolyte composition of the cell plays an active role in directing the formation and speciation of the soluble lithium polysulfides. Recently, new classes of electrolytes termed 'solvates' that contain stoichiometric quantities of salt and solvent and form a liquid at room temperature have been explored due to their sparingly solvating properties with respect to polysulfides. The viscosity of the solvate electrolytes is understandably high limiting their viability, however, cosolvents that thought to be inert to the solvate structure itself, can be introduced to reduce viscosity and enhance diffusion. In this work, Raman and NMR spectroscopy coupled with ab initio molecular dynamics simulations are used to study the unique solvation structure of 1,1,2,2-tetrafluoroethyl 2,2,3,3-tetrafluoropropyl ether as co-solvent in solvate $(MeCN)_2$?LiTFSI electrolyte that used in Li-S battery. The underlying design rules and implications to Li-S battery performance will be discussed.

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