Specific ion effects in carbonate-based energy storage materials

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Abstract.
Organic liquids are key components in modern battery materials that are of high importance for energy storage. This talk will summarize recent classical and quantum simulations of carbonate liquids (ethylene carbonate, propylene carbonate, and glycerol carbonate) that examine the structure and dynamics of the complex fluids. By comparing and contrasting the classical and quantum simulations, the accuracy of the classical models can be assessed. Differences between the models reflect the importance of polarization and charge transfer in the liquids. Specific ion effects on the structure of the liquids will also be discussed, as well as the impact of hydrogen bonding occurring in glycerol carbonate. The results will be compared with recent experimental efforts that measure solution structural, thermodynamic, and transport properties. The simulations give insights into the molecular level features that impact the measured properties.