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POS-26 The effect of 1,3-Dimethyl-2-imidazolidinone (DMI) as an additive in Lithium-ion cells.

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Improving the energy density, cost and lifetime of current lithium-ion batteries is vital for the electric vehicle industry and for grid energy storage. It is known that the composition of the electrolyte solution in lithium-ion batteries can dramatically affect their performance. For that reason, it is common to add a small amount of additives to the electrolyte solution to limit impedance growth, decrease the cell voltage drop during storage, and extend the cycling lifetime of the cells or to reduce the formation of gases inside them. In this work, a new electrolyte additive named 1,3-dimethyl-2-imidazolidinone (DMI), a molecule with a structure and a dipole moment similar to the better-known ethylene carbonate (EC) molecule, has been evaluated in cells with or without the co-additive vinylene carbonate (VC). This work combines a variety of experimental and theoretical methods, including differential capacity analysis (dQ/dV) and density functional theory (DFT) calculations, to explore the chemical effects of DMI in full lithium-ion pouch cells. It is found theoretically that DMI doesn't reduce or oxidize inside the voltage operational window of lithium-ion cells. In fact, the reduction and oxidation potentials of DMI are found to be -0.63 V vs Li/Li⁺ and 4.57 V vs Li/Li⁺, respectively. Furthermore, our experimental data suggest that the electrochemical impedance of cells with DMI as an additive strongly depends on the cathode composition. This effect is unusual, in that it is not typically seen for other additives, such as VC. This significant difference in impedance for different cathode composition is interesting in the sense that it could be used to study and better understand the physical and chemical properties of the cathode electrolyte interface (CEI), which is much less studied than its anode analogue, the solid electrolyte interface (SEI). Adding the co-additive VC increase the electrochemical impedance and decrease the cell voltage drop during storage.

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