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Temperature-dependent Crystal Structure of Dimethyl Carbonate

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The performance and safety/stability of Li-ion batteries (LIBs) can be enhanced by optimizing the charge-storing electrode materials and/or the charge transfer-mediating liquid electrolytes. In LIB research, the major focus has been on the electrode subsystem, while liquid electrolytes are studied much less [1].

Upon cooling of LIBs to investigate their performance at low temperatures, a series of Bragg reflections has been observed, which was assigned to the freezing of the liquid electrolyte [2]. Additional measurements reveal the development of long-range order in the model electrolyte mixture LP30 (ethylene carbonate (EC), dimethyl carbonate (DMC), and 1 M LiPF₆). To further study this evolving order, the individual components of the system must be examined. Of particular interest are insights close to ambient conditions, for such in situ LIB studies at sub-ambient temperatures.

This contribution outlines our efforts to crystallize DMC with minimized preferred orientation, in order to study the unit cell across the entire solid temperature range using neutron- and synchrotron-based powder diffraction techniques. Additionally, the datasets are complemented by x-ray single-crystal diffraction measurements.

[1] B. Flamme et al., Green Chem. 19, 1828-1849 (2017). (<https://doi.org/10.1039/C7GC00252A>)

[2] A. Senyshyn et al., Journal of Power Sources 282, 235-240 (2015). (<http://doi.org/10.1016/j.jpowsour.2015.02.008>)

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