Contribution ID: **43** Type: **Poster**

Temperature-resolved Crystal Structure of Ethylene Carbonate

Friday 6 December 2024 13:45 (3 hours)

For more than three decades, lithium-ion batteries (LIB) have been widely used as power sources for portable electronics and are of interest for electric vehicles and network applications (large-scale electricity storage). While there have been significant changes from the initial design of the LIB, the main solvents constituting the liquid electrolyte, responsible for the charge transfer between the electrodes, remained mainly unchanged [1]. An important class of solvents used in liquid electrolytes are linear and cyclic carbonates, because of the combination of physical/chemical properties in a mixture with two or more solvents with a lithium salt and additives [1]. Ethylene carbonate (EC), with its high dielectric constant [1] and ability to provide the protective SEI layer, is present in almost all commercial batteries, mixed with other solvents due to its high melting point [2].
After the determination of the crystal structure of EC from single crystals [3], this contribution presents room temperature data obtained by Neutron Powder Diffraction at SPODI (FRM II), temperature-dependent Neutron Powder Diffraction data from ECHIDNA (ANSTO) and Total Scattering and temperature dependent Powder X-Ray Diffraction data measured at P02.1 (DESY), showing the structural evolution from 3 K up to its melting point.
[1] G. Eshetu et al., Phys. Chem. Chem. Phys. 15, 9145-9155 (2013)
[2] J.-M. Tarascon & M. Armand, Nature 414, 359-367 (2001)
[3] C.J. Brown, Acta Cryst. 7, 92-96, (1954)

Primary author: WESTPHAL, Lea (TUM/MLZ)

Co-authors: SENYSHYN, Anatoliy; PORCHER, Florence (LLB, CEA/Saclay (France)); AVDEEV, Max (Australian Nuclear Science and Technology Organisation); MÜLLER-BUSCHBAUM, Peter (TU München, Physik-Department, LS Funktionelle Materialien); Dr KOCHETOV, Vladislav (FRMII TUM); Dr BARAN, Volodymyr (DESY, FS-PETRA-D, P02.1)

Presenter: WESTPHAL, Lea (TUM/MLZ)

Session Classification: Poster Session

Track Classification: Structure Research