Contribution ID: **28** Type: **Poster**

Critical Review of symmetry and structure relationships in graphite intercalation compounds (GICs) and their practical use for lithium ion battery materials

Wednesday 8 December 2021 10:30 (1h 30m)

Graphite and materials made of graphite have historically been of huge technological importance due to their manifold interesting properties. High performance lithium-ion batteries (LIBs) typically use graphite-based anode materials. The energy storage is achieved through the reversible reaction of the graphite with lithium ions in an electrochemical intercalation reaction. When the material is completely transformed to the stage-1 compound with maximum lithium content, LiC6 is obtained. The transformation to LiC6 however is complex and between the two terminal points of this reversible reaction, many intermediate stages exist. The profound complexity and peculiarities of this "staging"reaction, especially in the Li-Graphite system however are not yet fully understood. Although a full understanding is imperative in order to control aging and cell performance characteristics of lithium ion batteries.
We have critically reviewed the existing binary stage-1 GIC structures and especially the Li-GIC structures from the ICSD-database. We review fundamental structural aspects like bonding distances and packing arrangements and explore their symmetry relationships applying group-subgroup considerations. Our findings can be used to improve the understanding of the intermediate stages occurring during the electrochemical intercalation of lithium ions in LIBs and to enhance the analysing of measured neutron data.

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Session Classification: Poster Session II

Track Classification: Structure Research