



Contribution ID: 525

Type: Poster Presentation

Impact of Morphology on Lithium Transport and Structural Evolution in Li_2MnO_3 Cathode Materials

Li_2MnO_3 , a promising cathode material for high-performance energy storage, was synthesized in nanosphere, nanoporous, and bulk morphologies using the amorphization and recrystallization technique. The influence of morphology on the structural evolution and electrochemical behavior of Li_2MnO_3 was investigated focusing on its impact on lithium-ion mobility and structural stability during delithiation. All structures exhibited intrinsic defects, which intensified with delithiation, affecting lithium-ion transport. X-ray diffraction (XRD) analysis revealed progressive peak broadening accompanied by a slight rightward shift of the peak at 38° , suggesting cation mixing and increasing structural disorder as lithium content decreased. These changes reflect the challenges in maintaining structural integrity during cycling. Further analysis showed that delithiation led to pore size enlargement in the nanoporous morphology, while a structural transformation from the layered phase to a spinel-like configuration occurred, particularly from the $\text{Li}_{1.25}\text{MnO}_{2.25}$ compositions onward. This transition, along with significant lattice disruption, points to complex degradation mechanisms that impact material stability. Among the morphologies, the nanosphere exhibited the highest radial distribution function ($g(r)$) values, indicating improved local ordering favorable for ion movement. Diffusion coefficient analysis further confirmed enhanced lithium-ion transport in the nanosphere structure. These results suggest that morphology plays a critical role in determining the structural stability and electrochemical behavior of Li_2MnO_3 -based cathodes, offering insights that can inform the design of improved nanostructured materials for lithium-ion battery applications.

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Session Classification: Poster Session

Track Classification: Track A - Physics of Condensed Matter and Materials