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Contribution ID: **45** Type: **Student Micro-talk**

Monitoring the Structural Change and Lithium Diffusion Rate on Li-Mn-O Nanoporous Materials during the Discharge Process

Spinel LiMn2O4 has attracted tremendous attention and is the Li-ion battery research hotspot for the potential facilitation of a constant energy supply and storage. This is due to LiMn2O4 being cost-effective, having good structural stability with improved safety conditions and environmental affinity. Furthermore, it has an excellent rate performance with 3D Li+ diffusion channels. However, spinel LiMn2O4 suffers from a severe loss of specific capacity and voltage fade; especially, under high temperatures operations, hampering its commercial applications in lithium batteries. Porous structures at the nanoscale shorten the Li-ion diffusion length between the electrolyte and the electrode. This suggests that they can provide a large surface area and pore volume for better interaction with the electrolyte and ionic diffusion, leading to enhanced electrochemical performance and mechanical stability. In this study, molecular dynamics simulations using the DL_POLY code were employed to perform all calculations yielding structural changes and the lithium diffusion for the Li-Mn-O nanoporous (75, 69 and 67 Å) at different lithium concentrations, Li1+xMn2O4, where $0 \leq x \leq 1$.Recrystallisation of the structures results in single and multiple grained materials with defects. Furthermore, the structures reveal the reduction of the Mn3O4 content with increasing lithium concentration, where Mn2+ atoms, retained tetrahedral tunnels are observed. Moreover, the pore sizes of the structures fluctuate with increasing lithium content. The nanoporous structures expand during the discharge process, however, their structural integrity is maintained since they are capable of flexing within their pores. The diffusion coefficients of lithium with increasing concentration and temperature show that the pore size of a material influence its diffusion rate; nanoporous 75 Å showed the highest lithium diffusion rate, followed by nanoporous 69 Å and lastly nanoporous 67 Å. Therefore, nanoporous structures can enhance the performance of Li-ion batteries since they have high diffusion rates and can adapt to structural changes that may cause damage to the battery material during the discharge process.
CHPC content:
Each job calculation begins execution and is complete using ncpus=24, mpiprocs=24 and walltime=48:00:00 on a normal node using the DL_POLY code 2.2 at the Lengau cluster.

Student?

Yes

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