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Variation of Statistical Ensembles to Optimise Complex Core-Shell Cathode Models: A Molecular Dynamic Approach

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The O3-type Li2MnO3 is one of the potential replacements of the expensive nickel and toxic cobalt-based cathode materials for the portable, high power and high energy density lithium-ion batteries. However, Li2MnO3 suffers structural instability during cycling. Surface coating of cathode materials has sparked attention and has modified most of the commonly used cathode materials. The O3-type Li2MnO3 layered has been investigated over the years as a coating material for other cathodes but never as the core material. The O2-type Li0.69MnO2 is of great interest because unlike other lithium manganese oxides, it does not transform into a spinel structure during cycling and its conductive property enables it to allow undisturbed movement of Li atoms during battery operation. This study explores firstly the tedious process of modelling and developing core-shell systems that are meant to serve as electrode material with coating interface. The second aspect of interest is optimising the simulation conditions for molecular dynamic simulations of these core-shell systems. A core-shell model of the Li2MnO3-Li0.69MnO2 system is presented and preliminary molecular dynamics results are demonstrated under different ensembles. The Li2MnO3-Li0.69MnO2 core-shell structure was slightly disordered under the ensembles NPT, NST, and NVT. The radial distribution function plots indicated the bonding length to be 2Ã between the manganese and oxygen from both the core and shell through the different ensembles.

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Yes

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MSc

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