Molecular Dynamics (MD) thermal simulations of molecular bridging across the cathode-separator interface in a Li-ion cell

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Abstract

While Li-ion cells show outstanding electrochemical performance, their poor thermal transport characteristics results in reduced performance as well as significant safety concerns. The heterogeneous interface between cathode and separator plays a vital role in the dissipation of heat within a Li-ion cell. Previous studies showed that the cathode-separator interfacial thermal resistance contributes around 88\% of total thermal resistance within the cell. In this research, thermal conductance across the cathode-separator interface is calculated using molecular dynamics simulations. Thermal transport in a pristine heterogeneous interface as well as interfaces functionalized with monolayers of APTES, nBTMS and MPTSM molecules is studied. The impact of molecular density and external pressure on the interfacial thermal transport is studied. It was observed that interfacial functionalization results in significant improvement in interfacial thermal conductance, which is consistent with past experimental data. Molecular dynamics simulations presented here help validate past experimental measurements. Using 20 MPTSM molecules, 174\% improvement in thermal conductance was observed compared to bare interface. 2X improvement in 20 molecules of nBTSM by applying 100 bar pressure was observed compared to non-pressured of same system. These results highlight the key role of the cathode-separator interface in thermal transport within the cell, as well as the significant impact of functionalizing the interface to mitigate poor thermal transport in the Li-ion cell.