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The Diffusivity and Li^+ Conductivity of $LiTi_2(PO_4)_3$ Nanosphere for Solid State Battery Electrolytes

The NASICON-type $LiTi_2(PO_4)_3$ solid electrolyte is amongst the most promising electrolytes for solid-state batteries due to its broad electrochemical stability window and strong chemical durability. However, its relatively low ionic conductivity remains a major limitation for practical applications, hindering further development of $LiTi_2(PO_4)_3$-based technologies. Studies have shown that reducing the active particle size enhances solid-state electrolyte conductivity by increasing electrode-electrolyte contact and shorten the Li^+ diffusion path. In this study, molecular dynamics simulations are employed to investigate the diffusion coefficients of Li, Ti, P, and O atoms and the lithium-ion conductivity of the $LiTi_2(PO_4)_3$ nanosphere. The $LiTi_2(PO_4)_3$ nanosphere was generated using the METADISE code, and the temperature-dependent simulations were conducted under the NVT ensemble from 5 K to 2000 K. The diffusion coefficient increased with temperature for all atomic species, with a notable decline observed at 300 K, possibly caused by the lithium redistribution between the M1 and M2 sites that takes place at 270 K. Furthermore, the lithium-ion conductivity of the $LiTi_2(PO_4)_3$ nanosphere at room temperature was determined to be 5.297×10^{-1} S/cm using the Nernst-Einstein equation, which is three orders of magnitude higher than that of the bulk material (2.41×10^{-4} S/cm). The findings of this study indicate that indeed reducing the particle size of materials can enhance their performance since the nanosphere architecture of the $LiTi_2(PO_4)_3$ shows improved lithium-ion transport properties, potentially improving the performance of solid-state batteries.

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