

A Molecular Dynamics Simulation of the Transport Properties of Molten ($\text{La}_{1/3}$, K)Cl

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Molecular dynamics simulations of molten ($\text{La}_{1/3}$, K)Cl at 1123 K have been performed in order to investigate the correlation between simulated dynamical properties such as the self-exchange velocity (v), the self-diffusion coefficient (D) and the electrical conductivity (κ) and the corresponding experimental values. The simulated results revealed that v and D of potassium decrease with increasing mole fraction of lanthanum, as expected from the experimental internal cation mobilities, b . The decrease of b_{K} , v_{K} and D_{K} is ascribed to the tranquilization effect by La^{3+} , which strongly interacts with Cl^- . In contrast, b_{La} , v_{La} , and D_{La} increase with increasing concentration of La^{3+} . The distorted linkage of the network structure of $[\text{LaCl}_6]^{3-}$ units was disconnected with increasing the concentration of the alkali chloride. This might be attributed to the stronger association of La^{3+} with Cl^- due to the enhanced charge asymmetry of the two cations neighboring Cl^- . The sequence of the calculated v 's, D 's, and κ 's is consistent with those of the referred experimental results.

Key words: Internal Mobility; Molten Salts; Molecular Dynamics Simulation;
Self-exchange Velocity.