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The Effect of Internal Electrical Ion Mobility on Molten Salts through Atomistic Simulations

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Abstract : Binary and ternary mixtures of molten salts are excellent thermal energy storage systems and have been widely used in commercial tanks both in nuclear and solar thermal applications. However, the energy density of the commercially used mixtures is still insufficient, and therefore, new systems based on latent heat storage (or phase change materials, PCM) are currently being investigated. In order to shed some light on the macroscopic physical properties of the molten salt phases, knowledge of the microscopic structure and dynamics is required. Several molecular dynamics (MD) simulations have been performed to model the thermal behavior of (Li,K)2CO3 mixtures. Up to this date, this particular molten salt mixture has not been extensively studied but it is of fundamental interest for understanding the behavior of other commercial salts. Molten salt diffusivities, the internal electrical ion mobility, and the physical properties of the solid-liquid phase transition have been calculated and compared to available data from literature. The effect of anion polarization and the application of a strong external electric field have also been investigated. The influence of electrical ion mobility on local composition is explained through the Chemla effect, well known in electrochemistry. These results open a new way to design optimal high temperature energy storage materials.

Keywords : atomistic simulations, thermal storage, latent heat, molten salt, ion mobility
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