Molecular Dynamics Simulation of Molten Alkali Nitrates

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Molecular dynamics (MD) simulations have been performed for several pure alkali nitrate melts. Special attention was paid to the examination of the interaction potential: macroscopic quantities like pressure were calculated and compared with real values. To improve the results the commonly used potential for alkali nitrates (Coulomb pair potential and Born-type repulsion) has been extended by a short-range-attraction term to meet the real behaviour of the liquid.

With these improved potentials, simulations of pure $LiNO_3$, $NaNO_3$, KNO_3, and $RbNO_3$ have been performed with special regard to the influence of size and mass of the cations on the transport effects to show analogies to isotope effects. The calculated self diffusion coefficients (SDC) have been compared to results obtained with the NMR spin echo method.

Key words: Simulation; Molecular Dynamics; Interaction Potential; Alkali Nitrate; Melt.