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Molecular dynamics study of the influence of temperature on Ti7/LiCl structure

In this study, we employ computational modelling techniques to explore the structural behaviour of the Ti7 cluster in LiCl as a medium of interaction (problem size: 432 – 1024 atoms). We employed the molecular dynamics code (DL_POLY) using a core count of 48 and 24:00 wall time on a normal queue, to understand the Li-Cl, Ti-Cl, Li-Li, Li-Ti and Cl-Cl interactions of the system at a temperature range of 300 K – 1000 K. The LiCl structure was validated by comparing the lattice parameters of LiCl with experimental data and were found to be in good agreement. We observed that the interatomic Buckingham potentials used reproduced the structure to within 1% in agreement with experimental data. Furthermore, the radial distribution functions for the Ti7/LiCl system, show a phase transition from solid to liquid in the temperature range of 600 K - 800 K. The results of this study provide insight into understanding the growth of titanium in salt mediums, significant for maximizing titanium metal production.

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