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## Simulation of LiCl as a salt medium: a rigid ion and shell model comparison

Titanium in its metal and powder form can be produced through thermochemical processes involving the reduction of a precursor such as titanium dioxide. However, the reduction process occurs extremely fast and results in the agglomeration of crystalline particles. This reduction process occurs in the presence of alkali metal and alkali earth metal salt mediums. In this study, we employ computational modelling techniques to understand how we can maximize titanium production for industrial use. We employed the DL\_POLY code using a core count of 48 and 24:00 wall time on a normal queue, to calculate the entropy and Gibbs free energy for the LiCl (rigid ion and shell models) structure. The behaviour of atoms and the spontaneity of the structure was determined in a temperature range of 300 K – 1000 K (problem size: 216 atoms). It was observed that the entropy alternates between a decrease in disorder and an increase in disorder of atoms suggesting a phase transition. Furthermore, the Gibbs free energy calculations indicated that LiCl (shell model) is a favourable medium. These results provide an insight into understanding the reactions and interactions of titanium clusters with salt mediums in titanium production processes.

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