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Structural analysis of Ti/LiCl at different temperatures

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In this study we explore an alternative way to maximize Ti production by using LiCl salt. We employed the DL_POLY code to understand the interaction of LiCl at various temperatures in order to achieve Ti that has good properties at high temperatures. The LiCl structure was validated using available experimental and ab initio structural data such as elastic constants. The molecular dynamic results of LiCl show that the simulation used is a reliable model of a bulk alkali halide and this model is sufficient to set an environment that will allow to investigate the evolution of titanium. Furthermore, the RDF's of the Ti/LiCl structure depict a change in the morphology of the system for all interactions as the temperature is increased. The results of this study might give us more insight on the growth of titanium in salt mediums and on whether this salt can possibly be used to maximize Ti production.

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Yes

Level for award
 (Hons, MSc,
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MSc

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