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Evaluating the growth/evolution of Ti5 cluster in LiCl medium

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Titanium can be produced as both a metal and in powder form. It finds applications in various industries such as in medical and aerospace, where the fabrication of components with excellent corrosion and high-temperature performance are significant. The titanium metal also plays a significant role in the titanium production process due to its desirable physical and chemical properties. Also, this process occurs in the presence of alkali metal and alkali earth metal salt mediums. Recent experimental studies are on testing the lithiothermic part of the titanium formation process, however, the small titanium clusters are thermodynamically unstable. In this study, classical molecular dynamic calculations were performed to understand the growth/evolution of the small titanium Ti5 cluster after interactions with LiCl medium. The DL_POLY code was used to evaluate the temperature dependence of the structure. Furthermore, the stability of the cluster was evaluated using the CASTEP code. It was found that the cluster maintains its trigonal bipyramid geometry at the temperature range of 100 K – 2000 K. Moreover, the cluster was observed to show growth patterns, indicated by the absence of bonding between atoms. The results of this study might give us more insight into the growth/evolution of titanium in salt mediums.

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Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

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