Contribution ID: **80**

Type: **Poster (Chemistry SIG)**

Computational modelling studies of Ti-cluster formation in LiCl

The Molecular Dynamics calculations of the LiCl and Li-Cl-Ti systems were achieved by utilizing various codes of MD simulations at the CHPC.

The Thermodynamic properties and temperature dependence calculations of the structures were achieved by utilizing the DL_POLY code.
Application code: DL_POLY
Problem size: 216 – 1024 atoms
Core count: 48

Presenter Biography

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