

(Research Article)

Investigation of phonon modes and electron charge density of Ti_2InC By using density functional theory

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Abstract

In this paper, phonon modes and charge density of titanium indium carbide compound are calculated. The calculations have been performed using Pseudopotential method in the framework of density functional theory by the Quantum Espresso package. The number of phonon modes has been reduced from 24 to 16 due to the symmetry of the crystal. Also, the charge density diagram shows a strong bond between carbon and titanium atoms and a weaker bond between titanium and indium atoms. The calculations are in good agreement with other results.

Keywords: Ti_2InC , Density functional theory, Pseudopotential, Quantum espresso, Phonon modes.

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