



Contribution ID: 209

Type: Poster

Ab initio study of the crystal structures and mechanical properties of some late transition-metal nitrides

The crystal structures and mechanical properties of some late transition metal-nitrides at different stoichiometries and different structures have been investigated using first-principles density-functional theory. Obtained results were compared with theory and with experiment whenever possible.

Primary author: Mr SULEIMAN, MOHAMMED (University of the Witwatersrand)

Co-author: Prof. JOUBERT, DANIEL (University of the Witwatersrand)

Presenter: Mr SULEIMAN, MOHAMMED (University of the Witwatersrand)

Track Classification: Track G - Theoretical and Computational Physics