Contribution ID: **252** Type: **Oral Presentation**

The effects carbon and boron on the T-MnAl alloy properties employing the first principle approach.

Monday, 4 July 2022 16:15 (15 minutes)

The development of permanent magnets without rare-earth elements has gained a lot of attension. The T-phase MnAl alloy has gained particular attention due to the low cost of materials required. The density functional theory (DFT) within the generalized gradient approximation (GGA) was used to perform first-principle calculations, to study the T-MnAl alloy. The effects of carbon and boron on the electronic and magnetic properties of T-MnAl alloy were studied. The spin Orbital magnetic moments of Mn, C, and B ions were found to be opposite to each other, which is in agreement with Hund's rule. The total spin magnetic moments were found to be lower than that of the total orbital magnetic moment.

Apply to be considered for a student ; award (Yes / No)?

yes

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

MSc

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