Contribution ID: **431** Type: **Poster Presentation**

Investigation of structural and electronic properties of BCC Ti4V4Cr4Mn3Al high entropy alloy

Hydrogen generation is predicted to replace fossil fuels in the future due to its capacity to manufacture low-carbon hydrogen through electrolysis with renewable electricity. Storage remains a challenging issue that impacts safe end utilization of hydrogen as fuel as well as its distribution and delivery. Hydrogen storage criteria for solid-state fuel cell applications include high volumetric storage capacity, good heat transmission, recharge time, and reasonable charging and discharging temperatures. Recently, high entropy alloys (HEA) enabled extensive compositional freedom for the creation of advantageous simple solid solution phases for hydrogen storage. In this work first principle computations are employed to investigate the structural, electronic and mechanical properties of Ti4V4Cr4Mn3Al HEA. It was found that Ti4V4Cr4Mn3Al HEAs compounds are energetically stable with heats of formation value greater than zero. Moreover, it was observed that the computed stability vary with with HEAs phase formation. The Ti4V4Cr4Mn3Al HEAs was found to the most stable with the BCC phase and lattice parameter a=b=c 5.86Å. . Density of states and elastic constant were computed to investigate the electronic and mechanical properties. It was found that the Ti4V4Cr4Mn3Al satisfy mechanical stability criteria for BCC phase.

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Session Classification: Poster Session

Track Classification: Track A - Physics of Condensed Matter and Materials