Contribution ID: **244** Type: **Poster Presentation**

Effect of Co addition on the structural, electronic and magnetic properties of Fe16N2 employing first principles approach

Thursday, 11 July 2019 15:00 (2 hours)

Improvements in energy efficiency and reduction of greenhouse gas emissions have been some of the central topics in recent years in environment and climate change. The advantages of using permanent magnets in many different types of electromagnetic drive and static magnetic field applications are compelling. It seems demand is bound to increase substantially in coming years. There are significant challenges associated with coming up with new alloys or composite materials that can be used for bulk permanent magnets with an energy product in excess of 460 kJ m−3. In this study, first-principles approach employing the density of states within the generalised gradient approximation is employed. The structural, electronic and magnetic properties of Fe16-xN2Co for the development of permanent magnets are investigated. Firstly, geometry optimization was performed to reach the equilibrium state of the structures and the results compared well with the available experimental results. Interestingly the density of states at the Fermi level decreases suggesting the stability of Fe16N2 with Co addition.

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

no

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

no

Primary author: Dr MODIBA, Rosinah (CSIR)

Co-author: Prof. NGOEPE, Phuti (University of Limpopo)

Presenter: Dr MODIBA, Rosinah (CSIR)

Session Classification: Poster Session 2

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