Contribution ID: **500** Type: **Oral Presentation**

Effect of Li composition on HCP to BCC phase transformation in ultra-lightweight binary Mg-Li alloys: an ab initio study

Thursday, 12 July 2012 11:00 (20 minutes)

Abstract content
   (Max 300 words)

Density functional theory based first-principles total energy calculations are used to determine the lithium concentration dependence of equilibrium lattice parameters, densities, binding and mixing energies (phase stability) and elastic propertis of binary random Mg1-xLix alloys spanning the 0 to 30 atomic percent Li concentration range, in the HCP, FCC and BCC structures. A model for predicting phase stability and elastic properties of random alloys is proposed. The Li composition that induces crystal structural changes leading to crucial HCP to BCC transition are analysed.

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

Yes

Level for award
 (Hons, MSc,
   PhD)?

PhD

Main supervisor (name and email)
and his / her institution

Phuti Ngoepe
Phuti.Ngoepe@ul.ac.za
University of Limpopo (Turfloop Campus)

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

Primary author: Mr PHASHA, Maje (CSIR)

Presenter: Mr PHASHA, Maje (CSIR)

Session Classification: DCMPM2

Track Classification: Track A - Division for Condensed Matter Physics and Materials