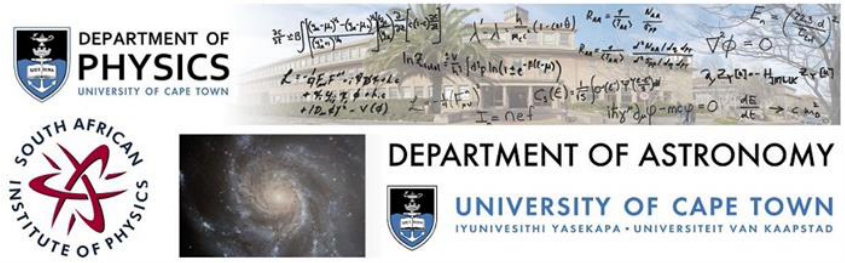

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Ab – initio study of transition metals impurities and stability of complexes in Ge.

Tuesday, 5 July 2016 16:10 (1h 50m)

Abstract content
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By means of density functional theory (DFT), we present ab-initio calculation of T(T: Cr, Mo, W, Mn and Fe) vacancy-interstitial complexes (T_{Ge}-V_{nGe}I_T, for n = 1,2 and 3) in Ge. The projector augmented wave (PAW) pseudopotentials within the generalized gradient approximation (GGA) was used for all the calculations. The structural properties and formation
energies of T_{Ge}-V_{nGe}I_T for the neutral charge state were obtained. Our results show that
under favourable energetic condition, vacancy-interstitial complex T_{Ge}-V_{nGe}I_T
will form with low formation energy. The formation energy show that the T_{Ge}-V_{nGe}I_T
is more energetically favourable for n = 1 and 2 than n = 3. The stability of the vacancy-interstitial complexes
were
obtained from their binding energies. For all T, the binding energies of the T_{Ge}-V_{Ge}I_T
are positive and stable. Except for the W and Mo, for the T_{Ge}-V_{2Ge}I_T
and T_{Ge}-V_{3Ge}I_T the binding energies for T are negative and the defect
complexes are likely to dissociate into smaller fragments.

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Main supervisor (name and email)
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Walter E. Meyer
wmeyer@up.ac.za
Univeristy of Pretoria

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Primary author: Mr IGUMBOR, Emmanuel (University of Pretoria)

Co-author: Dr MEYER, Walter (University of Pretoria)

Presenter: Mr IGUMBOR, Emmanuel (University of Pretoria)

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