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

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**Abstract content** **&nbsp;** (Max 300 words) **<br>** **<a href="http://events.saip.org.za/getFile.py/?target="\_blank">Formatting &** **<br>** **Special chars</a>**

By means of density functional theory (DFT), we present *ab-initio* calculation of T(T: Cr, Mo, W, Mn and Fe) vacancy-interstitial complexes ( $T_{\text{Ge}}-V_{\text{nGe}}I_{\text{T}}$ ), 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  $T_{\text{Ge}}-V_{\text{nGe}}I_{\text{T}}$  for the neutral charge state were obtained.

Our results show that

under favourable energetic condition, vacancy-interstitial complex  $T_{\text{Ge}}-V_{\text{nGe}}I_{\text{T}}$  will form with low formation energy. The formation energy show that the  $T_{\text{Ge}}-V_{\text{nGe}}I_{\text{T}}$  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  $T_{\text{Ge}}-V_{\text{Ge}}I_{\text{T}}$  are positive and stable. Except for the W and Mo, for the  $T_{\text{Ge}}-V_{\text{2Ge}}I_{\text{T}}$  and  $T_{\text{Ge}}-V_{\text{3Ge}}I_{\text{T}}$  the binding energies for T are negative and the defect complexes are likely to dissociate into smaller fragments.

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

yes

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

PhD

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

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

Yes

**Please indicate whether<br>this abstract may be<br>published online<br>(Yes / No)**

Yes

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