Contribution ID: **231** Type: **Presentation**

Energetic stability and magnetic ordering properties of 3d transition metals in diamond

The energetic stability and magnetic ordering properties of 3d transition metals in diamond are investigated using ab initio DFT methods. The divacancy is predicted to be the energetically most favourable site, with Cr, Mn, Fe, Co and Ni having the lowest formation energies. Spin polarised impurity bands are induced in the diamond band gap, suggesting that these elements are likely to order ferromagnetically when incorporated into diamond.

Primary authors: Prof. LOMBARDI, E B (Physics Department, University of South Africa(UNISA)); Mr BENECHA, E M (Physics Department, University of South Africa (UNISA))

Presenter: Mr BENECHA, E M (Physics Department, University of South Africa (UNISA))

Track Classification: Track A - Condensed Matter Physics and Material Science