Contribution ID: **406** Type: **Poster Presentation**

Predicting the Mo dopant induced electrical levels in Ge

Wednesday, 5 July 2017 17:10 (1h 50m)

In this report, an ab initio calculation results of the Mo dopant induced levels in Ge were presented. The density functional theory (DFT) with the Heyd, Scuseria, and Ernzerhof (HSE06) hybrid functional was used to calculate the minimum total energies for the Mo vacancy-complexes of Ge (V_{Ge} Mo_{Ge}) and Mo substitution in Ge (Mo_{Ge}). The formation energies of the first nearest neighbour (N1), second nearest neighbour (N2) and third nearest neighbour (N3) configurations for the V_{Ge} Mo_{Ge} as well as the Mo_{Ge} were obtained for charge states -2, -1, 0, +1, and +2. The calculated formation energies for the V_{Ge} Mo_{Ge} resulted to positive binding energies for the N1, N2 and N3 configurations. The N2 configuration is the most energetically favourable with a formation and binding energies of −0.14 and 0.06 eV, respectively. The Mo_{Ge} has a formation energy of −2.99 eV and induced electrical level which exhibits a negative-U ordering within the band gap of Ge. The (+1/-1) transition charge states induced by the Mo_{Ge} is a deep level lying at E_V + 0.31 eV.

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Session Classification: Poster Session 2

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