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Ab-initio studies of Tm³⁺ interstitial defects in Germanium (Ge) using Hybrid Functional HSE06

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Abstract content
   (Max 300 words)
Formatting &
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In this work we present ab-initio calculations results of Tm³⁺ interstitial defects in Germanium (Ge) in the frame work of density functional theory (DFT) using hybrid (HSE06) exchange correlation functional. We calculate the formation and transition levels energy of different configurations and their charge states of -2, -1, 0, +1 and +2. In all the configurations, our result shows that the formation energies are relatively low and stable, revealing the T configuration to be the most stable. While the T configuration did not have a positive-U the H exhibit some properties of positive-U . We found transition levels that behave as deep and shallow donor and deep acceptor. The transition levels of (0/-1) and (+1/0) lies at the mid region of the band-gap which give rise to small optical peak, while the transition level of (+1/+2) lies close to the valence band maximum.

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

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