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Electrical levels induced by thulium (Tm³⁺) in germanium: a hybrid density functional study

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In this work we present ab-initio calculation results for the Tm³⁺ interstitial, vacancy-interstitial complex (V_{Ge}-Tm³⁺_i) and substitutional (Tm³⁺_{Ge}) defects as determined by using the Heyd, Scuseria, and Ernzerhof (HSE06) hybrid functional. We calculated the formation energies and the charge state transition levels of different configurations. Our results show that the Tm³⁺_i exists in both the hexagonal and tetrahedral configuration with low formation energy. The interstitial atom is most energetically favourable at the tetrahedral site. The formation energies for the V_{Ge}-Tm³⁺_i and Tm³⁺_{Ge} were as low as 0.84 eV. The most energetically favourable defects were the V_{Ge}-Tm³⁺_i in the axial configuration and the Tm³⁺_{Ge}. The Tm³⁺_{Ge} and V_{Ge}-Tm³⁺_i introduced a single acceptor &epsilon(0/-1) charge state transition level that was positioned deep in the middle of the band gap. The majority of the levels induced by the defects under investigation were either shallow donor or acceptor level lying close to the band gap edges. The charge state thermodynamic transition levels revealed that the vacancy-complex V_{Ge}-Tm³⁺_{Ge} induced shallow levels in the band gap. The V_{Ge}-Tm³⁺_{Ge}displ evidence of a single donor level &epsilon(+1/0) and an acceptor level &epsilon(-1/-2) within the band gap. Charge state controlled metastability was exhibited by the V_{Ge}-Tm³⁺_{Ge}.

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