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Ab initio studies of Split<110> and Tetrahedral Di-interstitials of Germanium (Ge) using Hybrid functional HSE06

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As a result of its narrow band gap, high carrier mobility and low voltage operation the application of Germanium (Ge) as a promising material for complementary metal-oxide semiconductors (CMOS) technology is attracting attention recently [1]. Studies on Several defects including self-interstitials, interstitials, vacancies and vacancy complexes [2-3] have been carried out. For Silicon, various interstitials and vacancies including mono-, di- and tri- has been studied[2], Ge mono-interstitials using local density approximation(LDA), generalized gradient approximation (GGA) was reported[3], but none have been studied on mono- and di-interstitials of Ge using HSE[4]. In this work we present ab-initio calculations results of Ge Tetrahedral (TT) split<110> (SP10) and split<110>/Tetrahedral (SPT) di-interstitials configurations in the frame work of density functional theory(DFT) using hybrid functional (HSE06)[4] exchange correlation functional. The formation and transition level energies of defected configurations charge states of -2, -1, 0, +1 and +2 were obtained. Depending on the Fermi level, the formation energies shows that the SP10 is less favourable than T while the combination of SPT forms the most stable defect. We find (+1/+2) transition charges states level of TT to be 0.76 eV above valence band maximum (VBM) and (+1/+2) for (SPT) configurations to be 0.72 eV above VBM. These di-interstitials exhibited the properties of shallow and deep donor at (+1/+2) above the Fermi level depending on the configurations. We compare this result with calculation of di-interstitials in silicon and available experimental data.

Are you currently a postgraduate student? (Yes/No)

yes

At what level of studies are you currently? (Hons/MSc/PhD)

PhD

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