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NATURAL AND
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An Ab-initio Study into possible metastability of the Antimony-vacancy (Sb - V) complex in Germanium.

Wednesday, 6 May 2015 13:30 (1h 30m)

We are investigating the possibility of the Antimony-Vacancy complex (E-center) using the Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional within density functional theory (DFT). The results are then compared to the predictions we obtained to experimental observations. We have in the past observed interesting results for the similar case of metastability in the Boron – Vacancy complex in silicon and wish to extend this research further to the Antimony-Vacancy complex in Germanium. We investigate the dependencies of the formation energy of the complex to the position of the Germanium vacancy to respect to the substitutional Antimony within the supercell. We examine the ability of the HSE06 functional to accurately predict the thermodynamic charge transition levels and whether or not charge-state controlled metastability exists in that of the Sb-V complex. The nearest neighbor and next nearest neighbor configurations of the Sb-V complex were also examined to give a greater understanding of the nature of this defect.

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

Yes

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

Msc

Please provide the name and email address of your supervisor.

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