Contribution ID: **440** Type: **Oral Presentation**

An ab-initio study of the metastability of the boron-vacancy (B-V) complex in silicon.

Thursday, 2 July 2015 16:50 (20 minutes)

Abstract content
   (Max 300 words)
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We have investigated the metastability of the boron-vacancy (B-V) complex using PBE and the Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional within density functional theory (DFT) and compared it's predictions to experimental observations. Both the formation energies and thermodynamic transition levels of the defect were found to depend on the position of the silicon vacancy with respect to the substitutional boron. HSE06 predicted thermodynamic charge transition levels and charge-state controlled metastability of the B-V complex that was consistent with experimental observations. The nearest neighbor and next-nearest neighbour configurations of BV
complex were identified as the two metastable configurations of the defect complex.

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Session Classification: DPCMM

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