Contribution ID: **134** Type: **Poster (sponsored)**

Hybrid functional study of BiOi, BiCs, BiBsHi, and BiOiOi Complexes in Silicon.

Despite its technological importance, there are still many unanswered questions regarding the behaviour of defects in silicon. Oxygen, carbon and hydrogen are common impurities in Czochralski- (CZ-) grown silicon, therefore understanding the properties of ternary complexes of these impurities is technologically important. We show that the BiOi, BiCs, BiBsHi, and BiOiOi defects in silicon (Si) are stable and have determined their properties using density functional theory (DFT) using the Heyd, Scuseria, and Ernzehof (HSE) hybrid functional. The energy of formation and the thermodynamic charge transition levels of these defects were examined. All of the defects were found to have positive binding energy for the neutral charge state. Thermodynamic transition energy levels predict that BiCs has a donor level of (1/2) at Ev + 0.2 eV, and a double donor level (2/0) at Ev + 0.36 eV for BiOi, a shallow double donor level at Ev + 0.08 eV, and a sinle acceptor levelat Ec − 0.2 eV for the BiOiOi defect. Lastly a donor level (1/0) was found at Ev + 0.38 eV for the BiBsHi defect. The theoretical results were compared to available experimental data and a reasonable agreement was found.

Presenter Biography

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Session Classification: Poster session

Track Classification: Computational Chemistry