Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

The interaction of hydrogen donors with compensating acceptors in semiconducting oxides JOEL VARLEY[1], HARTWIN PEELAERS, ANDERSON JANOTTI, CHRIS VAN DE WALLE, University of California, Santa Barbara — Hydrogen is a common impurity that can act as a donor and an acceptor in a semiconductor, leading to a variety of behavior that may impact the desired performance. In one class of materials, wide-band-gap semiconducting oxides, the role of H has been strongly linked to n-type conductivity. In these systems H acts predominantly or exclusively as a shallow donor as an interstitial or while substituting on an O site. In addition to the resulting n-type conductivity, the incorporation of H or other donor dopants also leads to an increase in compensating acceptor defects. The interaction of H with cation vacancies, the dominant acceptor impurity involved in compensation, has yet to be fully explored. Using first-principles calculations employing hybrid functionals, we investigate the complexes formed between cation vacancies and interstitial H donors. We report on the formation energies, binding energies, and vibrational frequencies of the hydrogenated cation vacancies in the transparent semiconducting oxides SnO2, In2O3 and Ga2O3 [1]. We find that H can interact strongly with vacancies in both atomic and molecular form, and can have a significant impact on the electrical properties of devices employing these oxides.

[1] J.B.Varley et al., J.Phys. Cond. Matter 23, 334212 (2011).

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Date submitted: 29 Nov 2011 Electronic form version 1.4