

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Hydrogen in anion vacancies of semiconductors¹ MAO-HUA DU, DAVID SINGH, Oak Ridge National Laboratory — Hydrogen typically terminates the dangling bonds around vacancies in semiconductors, thereby, partially or completely passivating the vacancies. However, it has been shown recently that hydrogen in anion vacancies of many semiconductors, such as ZnO, MgO, InN, SnO₂, and GaN, takes multi-coordinated structures and acts as shallow donors, providing *n*-type conductivity to the materials. We study the hydrogen in the anion vacancies of a series of II-VI and III-V semiconductors using density functional calculations. The results on these materials show that, in the anion vacancies of polar II-VI semiconductors, the hydrogen is usually anionic and is coordinated with more than one cation atoms as a result of the relatively high ionicity of the host materials. The hydrogen coordination number depends on the host anion size. On the other hand, in more covalent semiconductors such as some III-V semiconductors, the single cation-H bonding configuration may become most stable. In the anion vacancies of ZnX and CdX where X represents anions, hydrogen is typically amphoteric except for oxides, in which the small anion size prohibits the formation of the cation-cation bond that is required for the acceptor configuration.

¹This work was supported by the U.S. DOE Office of Nonproliferation Research and Development NA22.

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Date submitted: 21 Nov 2008

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