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Hydrogen multicenter bond in oxide and nitride semiconductors¹

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Hydrogen is a very reactive atom, occurring in virtually all organic and in many inorganic compounds. It can form a purely covalent bond, in which two hydrogen atoms share a pair of electrons in a two-electron two-center bond, as well as polar covalent bonds, such as in an H₂O molecule. In solids, hydrogen is usually considered as an interstitial impurity. In elemental semiconductors, such as silicon, hydrogen forms a three-center bond when located at the bond center. In compound semiconductors, hydrogen bonds to the anionic species in p-type material, and to the cationic species in n-type. Thus far, hydrogen in solids has been found to form chemical bonds with one, two, or at most three other atoms. Higher coordination numbers are exceedingly rare and have been reported only for clusters. In this talk we will show that hydrogen is capable of forming multicenter bonds in solids, occupying substitutional sites. As examples, we discuss substitutional hydrogen impurities in oxides (ZnO, MgO, SnO₂, TiO₂) [1,2] and nitrides (InN, AlN, GaN) [3]. Based on first-principles calculations we show that hydrogen replaces oxygen (nitrogen) and forms genuine chemical bonds with multiple metal atoms, in truly multicoordinated configurations. These multicenter bonds are surprisingly strong despite the large hydrogen-metal distances when compared to typical values in hydrogen two-center bonds. Hydrogen in the multicenter bond configuration is a shallow donor in a number of materials. In conducting oxides, it provides a consistent explanation for the observed dependence of electrical conductivity on oxygen partial pressure, thus resolving a long-standing controversy on the role of point defects in unintentional n-type conductivity [1,2].

[1] A. Janotti and C. G. Van de Walle, *Nature Materials* **6**, 44 (2007).

[2] A. K. Singh, A. Janotti, M. Scheffler, and C. G. Van de Walle, *Phys. Rev. Lett.* **101**, 055502 (2008).

[3] A. Janotti and C. G. Van de Walle, *Appl. Phys. Lett.* **92**, 032104 (2008).

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