Researchers discover hydrogen can form multicenter bonds

December 4 2006

Researchers at the University of California, Santa Barbara have shown that, under the right circumstances, hydrogen can form multicenter bonds, where one hydrogen atom simultaneously bonds to as many as four or six other atoms. Tested for hydrogen in metal oxides, the discovery could have a broad range of technological impact.

The research is available today in the advance online publication of *Nature Materials*.

Professor Chris G. Van de Walle and Project Scientist Anderson Janotti, both of the Materials Department of the College of Engineering at UC Santa Barbara, have shown that multi-coordinated hydrogen is a likely explanation for electronic conductivity in metal oxides. Metal oxides are widely used in everything from sunscreen to sensors.

Hydrogen, the simplest of the elements (consisting of one proton and one electron) is typically expected to exhibit simple chemistry when forming molecules or solids. Hydrogen atoms almost always form a single bond to just one other atom, leading to a two-center bond with two electrons. Exceptions to the rule are rare; there are only a few cases when hydrogen bonds simultaneously to two other atoms, forming a three-center bond.

Hydrogen can replace an oxygen atom and form a multicenter bond with adjacent metal atoms. For example, in ZnO, hydrogen equally bonds to the four surrounding Zn atoms, becoming fourfold coordinated. These

multicenter bonds are highly stable and explain previously puzzling variations in conductivity as a function of temperature and oxygen pressure. The results suggest that hydrogen can be used as a substitutional dopant in oxides, a concept that is counterintuitive and should be of wide interest to researchers.

Source: University of California - Santa Barbara