**Hydrogen in** **indium oxide and gallium oxide**

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Indium oxide, with a band gap of 2.7 eV, is widely used as a transparent conducting oxide. Gallium oxide, with a band gap of 4.8 eV, is also conductive and remains transparent into the UV, and (AlxGa1-x)2O3 alloys have even larger band gaps. Hydrogen is often introduced during growth or processing of the material; in fact, in the widely used technique of metal-organic chemical vapor deposition (MOCVD) hydrogen is present in the metal-organic precursors and often used as a carrier gas. It is therefore important to assess the impact of hydrogen on the properties of these materials. We address these issues using first-principles calculations based on density functional theory. In both In2O3[1] and Ga2O3[2] hydrogen acts as a shallow donor, i.e., it contributes to *n*-type conductivity, but its behavior changes in (AlxGa1-x)2O3 alloys.[3] Hydrogen can also interact with other impurities or defects in the material.

We have also studied diffusion. In monoclinic *b*-Ga2O3, the most stable phase, hydrogen diffusion is highly anisotropic. For protons, the migration barrier is as low as 0.28 eV along the [010] direction.[3] In In2O3, with the bixbyite structure,local hopping of the proton, corresponding to a realignment of the O-H bond, can also occur with a low activation energy of 0.24 eV; however, this process does not lead to long-range diffusion.[4] The long-range migration path of H+ in In2O3 can be decomposed into rotations of the proton around oxygen and jumps between two oxygen atoms, with a higher overall activation energy of 0.94 eV. We compare our results with recent experiments.

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