Structural trends and band gaps within the Al-Zn-O system

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Abstract

In an age of flat screens and solar panels, a decent and affordable transparent conducting oxide (TCO) is essential. Tin-doped indium-oxide (ITO) meets the technical demands, but is economically less attractive due to the scarcity of indium. A possible alternative is Aluminum-doped zinc-oxide (AZO), though its conductivity does not yet reach that of ITO. A better understanding of how the aluminum influences ZnO is necessary.

In this work, we have applied various structure prediction tools to the Al-Zn-O system. For a set of given stoichiometries, several crystal structures were determined that are either the ground state for that stoichiometry or close to the ground state. Although these materials do not appear in nature themselves, they serve as virtual experiments to observe how Al behaves in a ZnO matrix, at various concentrations. Extrapolation of the observed trends to the regime of low Al-concentrations provides new insight that is relevant for understanding AZO.

Next to structural information also the band gaps have been monitored over this set of metastable crystals, using both the PBE functional and the modified Becke-Johnson functional. Trends for both sets of bandgaps will be discussed.

Keywords: Transparent Conductive Oxides, AZO, structure prediction, band gaps.