

**MS14-2-3 Wurtzite-type nitrides and oxide nitrides: structural diversity and the effects of oxygen**  
**#MS14-2-3**
**J. Breternitz<sup>1</sup>, S. Schorr<sup>2</sup>**
<sup>1</sup>Helmholtz-Zentrum Berlin für Materialien und Energie - Berlin (Germany), <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie; Freie Universität Berlin - Berlin (Germany)

**Abstract**

Although solar cells are widely commercialised, the current dominant technology based on crystalline silicon suffers from the indirect bandgap of silicon. This dictates that such modules are comparably heavy, thick and inflexible. Substitutes, such as CdTe, Cu(Ga,In)S<sub>2</sub> or lead halide perovskites, on the other hand, contain very scarce elements – such as Te & In – or very toxic elements – such as Cd & Pb, which would prevent their large-scale use. Therefore, finding alternative semiconductor materials with suitable properties and their thorough characterisation remains a task of uttermost importance for the widespread use of renewable energies.

Herein, we emphasise on the class of ternary and multinary wurtzite-based nitride and oxide nitride materials.[1] Deriving from the hexagonal wurtzite-type, a plethora of different subgroup types are observed, typically through ordering of cations in these materials, and we will rationalise their relationships in the form of a Bärnighausen tree (figure 1).[2] As an example, we will highlight the structural relations on the example of Zn/IVN<sub>2</sub> (IV = Sn, Ge), materials that are hotly debated as solar absorber candidate. They crystallise in the orthorhombic β-NaFeO<sub>2</sub>-type (s.g. *Pna2*<sub>1</sub>) when the cations are ordered. Interestingly, cation ordering has been identified as one way to tune the bandgap of these materials, and which is unique to those ternary nitrides. A different cation ordering obeying Pauling's rules was proposed for Zn/IVN<sub>2</sub> in s.g. *Pmc2*<sub>1</sub> from computation.[3] This latter has nominally higher symmetry than the β-NaFeO<sub>2</sub>-type due to the smaller unit cell size. However, it is unlikely to form, due to the specific symmetry in this space group that undermines the driving force for cation ordering.[2]

In real systems, a variable degree of oxygen incorporation can hardly be avoided in nitride materials. The structural effects of oxygen and cation disorder resemble at first sight, and we will highlight how they relate to each other with the aid of neutron diffraction in the model system Zn<sub>1+x</sub>Ge<sub>1-x</sub>(N<sub>1-x</sub>O<sub>x</sub>)<sub>2</sub>. [4,5] In addition to the structural changes, the oxygen content also affects the bandgap, which narrows upon oxygen incorporation. Using bonding analyses based on DFT calculations, we will explain the oxygen induced bandgap narrowing as an upward shift of the conduction band that is due to orbital overlaps of the Zn(3d) with the O(2p) and N(2p) orbitals.[6]

**References**

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Selected subgroup structures of the wurtzite-type.

