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Bandgap tuning in ZnGeN2: Effective cation disorder control through oxygen incorporation.

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Growing concern over resource availability and toxicity are leading to a paradigm shift towards truly sustainable materials for photovoltaics. Zn-group IV-nitrides are one potential class of materials fulfilling these criteria, which adopt a wurtzite-type derived structure. The ternary nitrides were postulated to allow a unique bandgap tuning mechanism through cation disorder[1] in addition to cation alloying. Fully ordered structure $ZnGeN_2$ crystallises in a ß-$NaFeO_2$ type structure in a subgroup of the wurtzite type. Interestingly, incorporating oxygen into $ZnGeN_2$ also introduces an increased degree of disorder in the material.[2]

We present a detailed study of the degree of cation disorder in oxygen containing $Zn_{1-x}GeN_2O_x$ that is revealed through neutron powder diffraction. Studying samples with a variable degree of oxygen allows us to conclude on the role of oxygen and further comparing different samples of nominally similar composition allows to decorrelate the oxygen effect from intrinsic cation disorder. We will combine our results with optoelectronic and chemical properties of the materials and finally aim to answer the question, whether cation disorder exists independently of oxygen incorporation or is fundamentally linked to it.

[1] A.D. Martinez, A.N. Fioretti, E.S. Toberer, A.C. Tamboli, *J. Mater. Chem. A*, **2017**, *5*, 11418.
[2] J. Breternitz, Z.Y. Wang, A. Glibo, A. Franz, M. Tovar, S. Berendts, M. Lerch, S. Schorr, *Phys. Status Solidi A*, **2019**, 1800885.

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