

## Molecular Precursor for S-doped ZnO

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The fine-tuning of the electronic properties of semiconductors is an important task for potential practical applications. It is well documented that the exchange with elements containing a different number of valence electrons leads either to p- or n-doping<sup>[1]</sup>. However, also an iso-valence substitution leads to marked effects. It has been observed that the band-gap is an almost linear function of composition (e.g. for  $\text{GaN}_x\text{As}_{1-x}$ ) with the band-gap of the respective binary materials (GaN, GaAs) as the margins.<sup>[2]</sup> Interestingly, a different behavior has been observed for ZnO. When  $\text{O}^{2-}$  is substituted by  $\text{S}^{2-}$  an adsorption edge down to 2.6 eV has been reported which is unusual because the band gap of ZnO is 3.3 eV and of ZnS 3.6 eV.<sup>[3]</sup> The latter materials were prepared by radio-frequency reactive sputtering.

In the current contribution, our goal is the preparation and characterization of tertiary materials containing sulfur  $\text{ZnO}_{1-x}\text{S}_x$  using a molecular source. The octameric, organometallic compound  $[\text{MeZnS-}i\text{Pr}]_8$ <sup>[4]</sup> represents a single-source precursor for the preparation of ZnS materials. Depending on the reaction conditions, it is possible to obtain the cubic sphalerite and the hexagonal wurtzite structure in different ratio. However, the presence of oxygen leads directly to pure ZnO.

Therefore, the second approach is to dissolve the ZnS-precursor in a liquid single source precursor for ZnO ( $[\text{MeZnOEtOMe}]_4$ )<sup>[5]</sup>. Under similar conditions than before  $\text{ZnO}_{1-x}\text{S}_x$  nanopowders can be obtained successfully. The incorporation of sulfur causes a considerable shift of the ZnO reflexes. For higher  $\text{S}^{2-}$  concentration as well as for elevated temperatures phase separation into a ZnO and ZnS phases occurs.

Our next goal is the synthesis of a real single-source precursor for  $\text{ZnO}_{1-x}\text{S}_x$  materials. The first results using a precursor containing O and S in a 1:1 ratio will be presented.

### Literature:

[1] H. Wenckstern et al., *Progress in Solid State Chemistry*. **2009**, 37, 153-172. [2] Akitaka Kimura, C. A. Paulson, H. F. Tang, T. F. Kuech, *Appl., Phys. Lett.* **2004**, 84, 1489. [3] B.K. Meyer, A. Polity, B. Farangis, Y. He, D. Hasselkamp, T. Krämer, C. Wang, *Appl. Phys. Lett.* **2004**, 85, 4929. [4] G.W. Adamson, H. M. M. Shearer, *Chem. Commun.*, **1969**, 16, 897-898. [5] Polarz, S.; Orlov, A.; Hoffmann, A.; Wagner, M. R.; Rauch, C.; Kirste, R.; Gehlhoff, W.; Aksu, Y.; Driess, M.; van den Berg, M. W. E.; Lehmann, M. *Chemistry of Materials* **2009**, 21, 3889.