

Synthesis of a new ternary nitride semiconductor - Zn_2VN_3 :

A combinatorial exploration of the Zn-V-N phase space

Supplementary information

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A computationally-guided combinatorial PVD screening of the entire Zn-V-N phase space is performed, resulting in the synthesis of the previously unreported ternary nitride Zn_2VN_3 . [1]

Figure 1 outlines the workflow of the accelerated materials discovery and design approach used in this work. It includes the computational prediction using density functional theory calculations, a comprehensive combinatorial phase- and property screening, and finally the synthesis and characterization of single-phase wurtzite Zn_2VN_3 .

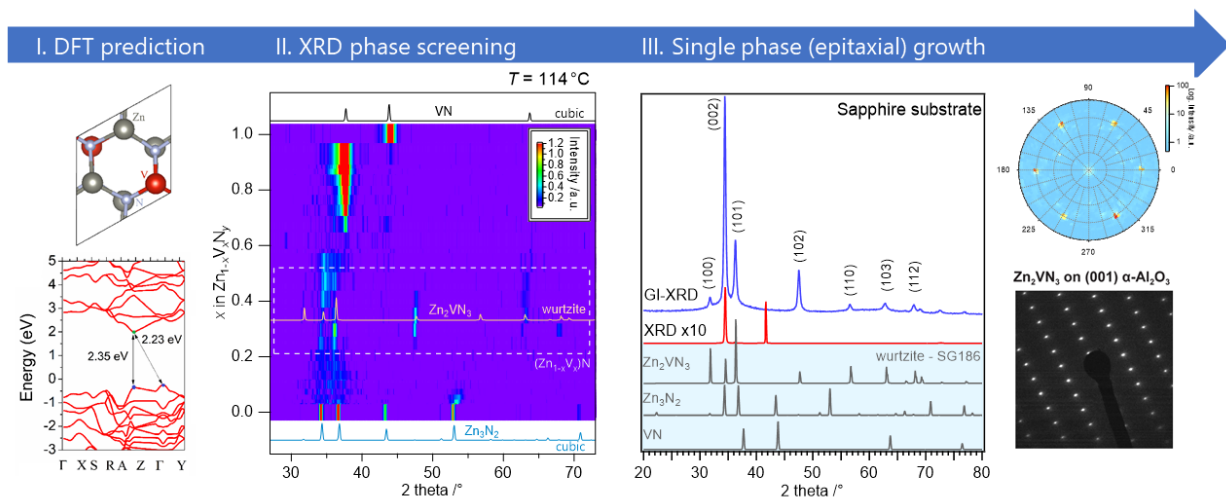


Figure 1: Workflow of the accelerated discovery and synthesis of Zn_2VN_3

[1] S. Zhuk *et al.* 2021 arXiv:2109.00365