

Abstract Submitted
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Origin of the anomalous piezoelectric response in wurtzite $\text{Sc}_x\text{Al}_{1-x}\text{N}$ alloys¹ FERENC TASNADI, BJORN ALLING, CARINA HOGLUND, GUNILLA WINGQVIST, JENS BIRCH, LARS HULTMAN, IGOR A. ABRIKOSOV², Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden, IFM COLLABORATION — We present the theory that reveals the origin of the observed anomalous enhancement of piezoelectric response in wurtzite $\text{Sc}_x\text{Al}_{1-x}\text{N}$ alloys [1]. Our first-principles calculations confirm that the 400% increase of the piezoelectric constant is an intrinsic alloying effect. The energy surface topology is found to be strongly influenced by the alloying, being elongated around the global minimum along $c=a$ direction. This leads to the large elastic softening along the crystal parameter c , and raises significantly the intrinsic sensitivity to axial strain resulting in the highly increased piezoelectric constant. The effect is particularly accentuated at intermediate compositions where the elongated double-minimum energy landscape is flattened due to the energy proximity of the wurtzite and so far experimentally unknown hexagonal phases of these alloys. Our observation provides a route for the design of materials with high piezoelectric response.

[1] F. Tasnadi, *et al.*, Phys. Rev. Lett. **104**, 137601 (2010).

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