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Structural Stability, Phase Transitions and Piezoelectric Anomalies in ordered $Sc_{0.5}Ga_{0.5}N$ Alloys. AHMAD ALSAAD, Department of Physical Sciences, Jordan University of Science and Technology — Local-density approximation (LDA) within density functional theory (DFT) and Berry phase approach within modern theory of polarization are performed to predict the structural and piezoelectric properties of ordered $Sc_{0.5}Ga_{0.5}N$ alloys under tensile and compressive in-plane strain. This alloy is found to exhibit a tremendous piezoelectric response, associated with a phase transition from nonpolar $p6_3/mcc(D_{6h})$ space group to a polar $p6_3mc(C_{6v})$ structure at fixed Ga and Sc compositions when continuously changing the experimental accessible parameter (i.e., the tensile and compressive strain). The mechanism of the effects behind such anomalies behavior are revealed and explained.

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