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Structural Phase Transitions induced by Compressive and Tensile Strains in Ordered $Sc_{0.5}Ga_{0.5}N$ and $Sc_{0.5}In_{0.5}N$ Alloys.[1] AHMAD ALSAAD, AHMAD AHMAD, Department of Physics, Jordan University of Science & Technology (JUST), Irbid-22110, Jordan, CONDENSED MATTER GROUP TEAM — Local-density approximation calculations (LDA) within density functional theory (DFT), Berry phase approach within modern theory of polarization and phonon calculations within the density functional perturbation theory are performed to predict the existence of breaking-symmetry structural phase transitions in ordered $Sc_{0.5}Ga_{0.5}N$ and $Sc_{0.5}In_{0.5}N$ alloys. It has been demonstrated that the existence of strain-induced structural phase transition leads to optimized optical, electronic, acoustic, and piezoelectric properties of ordered $Sc_{0.5}Ga_{0.5}N$ and $Sc_{0.5}In_{0.5}N$. In particular, It has been shown that ordered $Sc_{0.5}Ga_{0.5}N$ and $Sc_{0.5}In_{0.5}N$ alloys at fixed Ga, In and Sc compositions exhibit tremendous piezoelectric response (i.e., the e_{33} piezoelectric coefficient adopts a huge value as large as 8.3 C/m^2) as a function of the in-plane compressive and tensile strains. In addition, several optical, electric, acoustic anomalies will be shown and discussed. We also reveal the reason behind, and consequences of, these unusual properties associated with the biaxial strain-induced structural phase transitions.

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