Supplementary Information (SI) for Journal of Materials Chemistry C.

Supporting Information for

No Strain, No Piezoelectric Gain: Pushing Piezoelectric Boundaries via Strain Engineering in Composition-Tuned Wurtzite Scandium-Doped Aluminium Nitride

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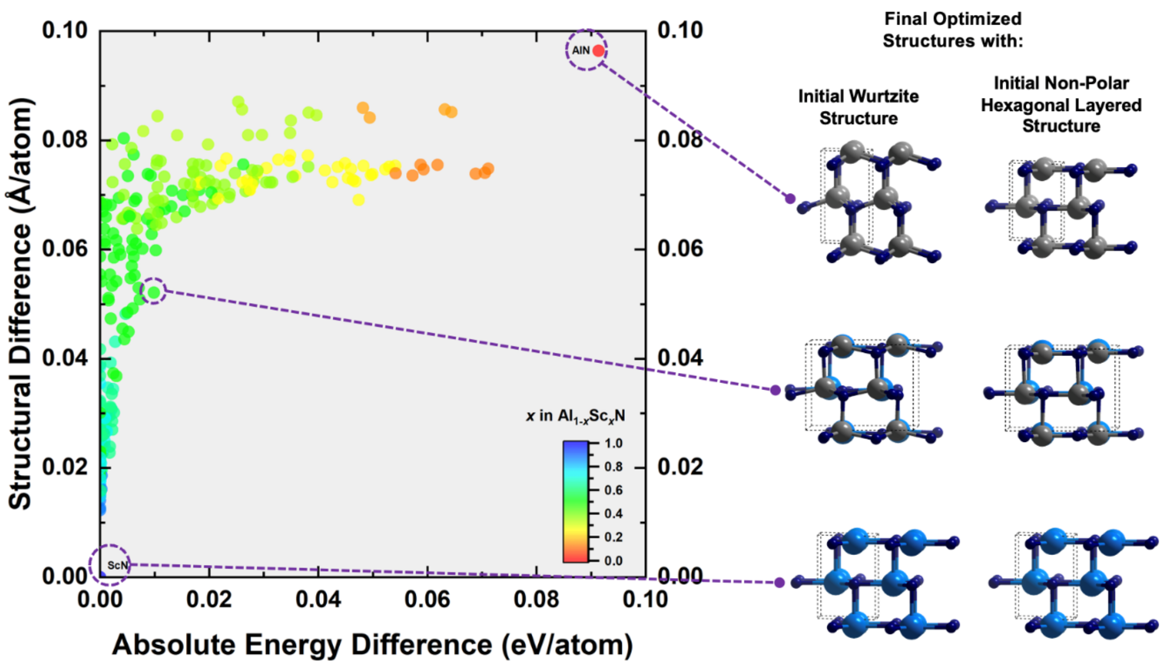

Figure S1. (Left) Plot of structural difference (as root sum squared distance or L-2 norm) versus absolute energy difference between wurtzite and non-polar hexagonal layered phases of $Al_{1-x}Sc_xN$ of particular alloy configurations. Pure AlN (x = 0) and ScN (x = 1) are identified and labelled on the graph to illustrate the range of structure and energy differences between the wurtzite and non-polar hexagonal layered phases. (Right) Final optimized structures with initial wurtzite and initial non-polar hexagonal layered structures for pure AlN (top), $Al_{0.5}Sc_{0.5}N$ (middle), and ScN (bottom).

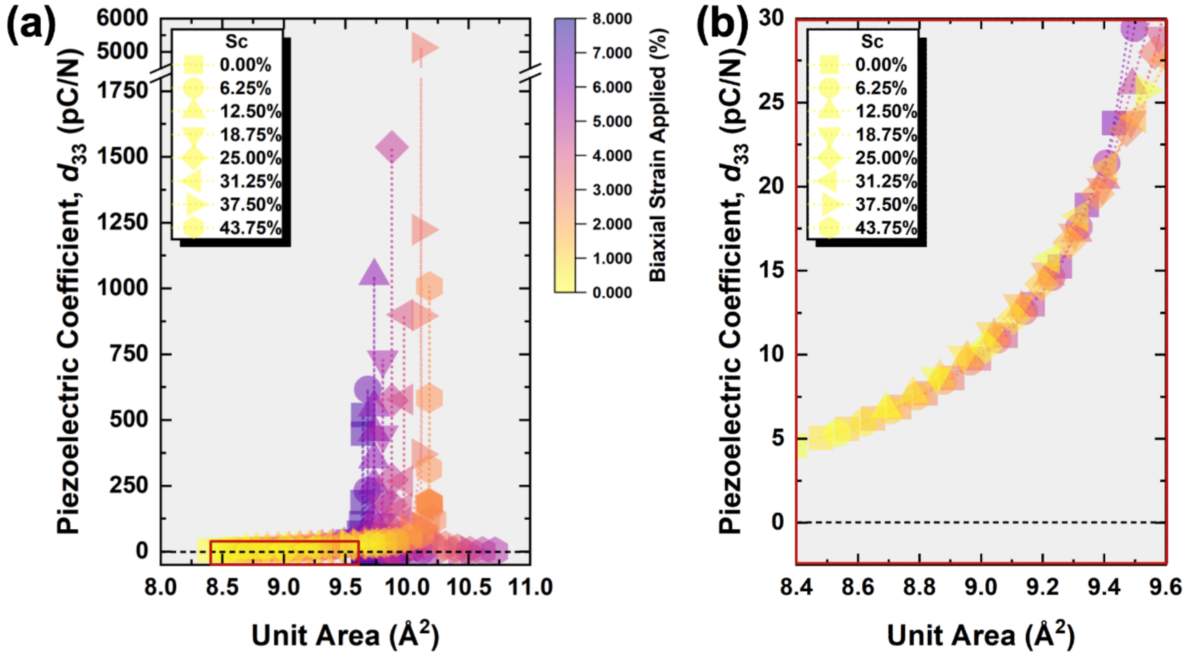

Figure S2. (a) Plot of piezoelectric coefficient, d_{33}, versus biaxial unit area for different Sc fraction, x, of $Al_{1-x}Sc_xN$ SQS supercells. (b) A magnified view of the region highlighted by the red rectangle in (a). The black horizontal dashed lines represent the abscissa.

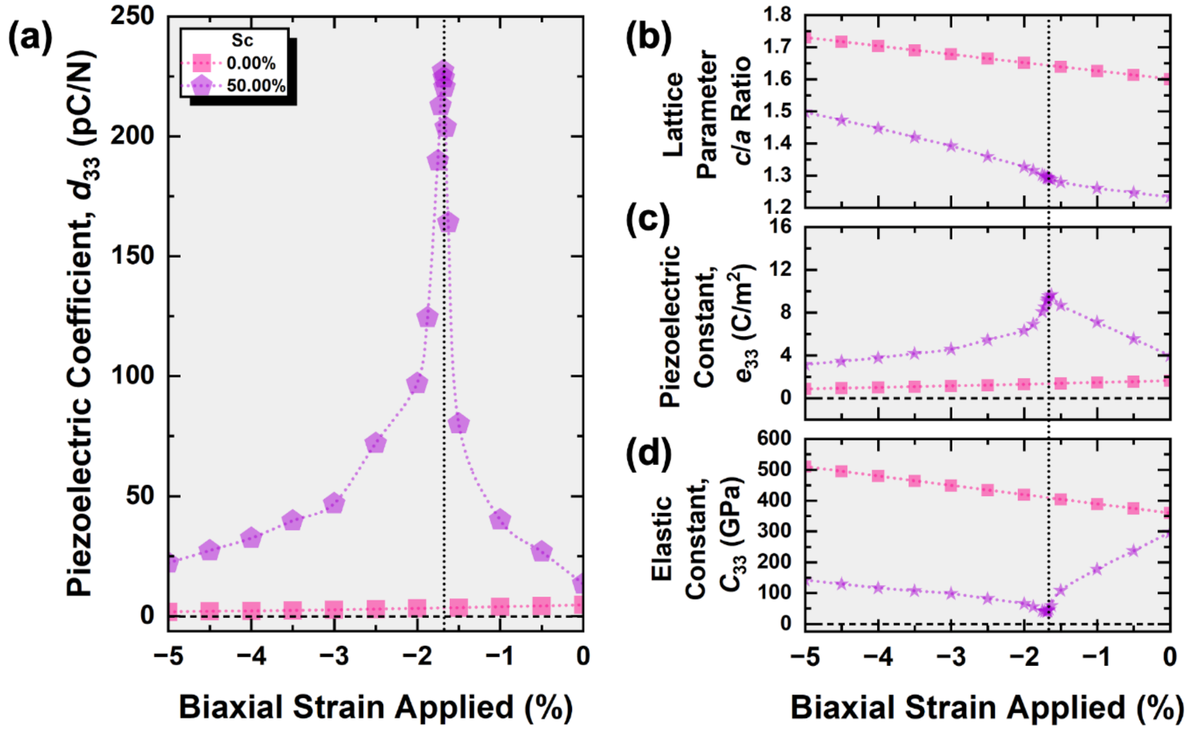

Figure S3. Plots of (a) piezoelectric coefficients, d_{33}, (b) lattice parameter *c*/*a* ratio, (c) piezoelectric constant, e_{33}, and (d) elastic constant, C_{33}, versus biaxial tensile strain applied for $Al_{0.5}Sc_{0.5}N$ SQS supercell and AlN. The negative values on the axis of the biaxial strain indicate that the biaxial strain is compressive. Black horizontal dashed line represents the abscissa. Vertical dotted line marks critical tensile strain of -1.69%.