Electronic structure of AlFeN films exhibiting crystallographic orientation change from *c*- to *a*-axis with Fe concentrations and annealing effect

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Supplemental:

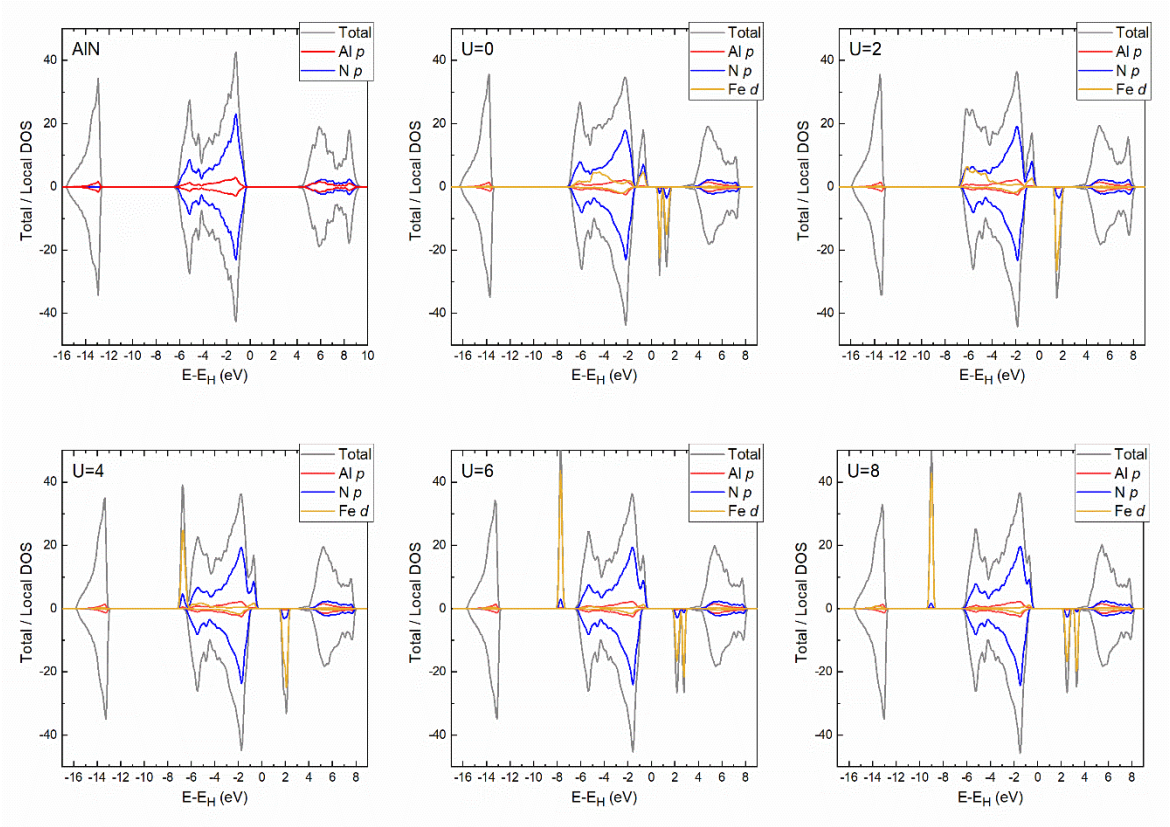

Fig. S1

Figures S1a-S1f show the calculated band structures using the VASP code for $Al_{33}Fe_3N_{36}$ for various Hubbard corrections (U) for Fe from U = 0–8. The zeros in each energy axis (E-E_H) are the highest occupied states by the electrons at ground state. In the N-*p* PDOS for U = 4, 6, and 8, a peak appeared just under the main component of VB between 0 and -6 eV. Because there was no corresponding peak in the XES, we chose U = 2 for Fig. 2f. To determine the Hubbard corrections (U) for Fe as well as Al and N, other experiments such as Fe *L*-edge XANES and XES include resonant XES and Al *K*-edge XES.