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LETTER

Strong ferroelectricity in one-dimensional materials self-assembled by superatomic metal halide clusters

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Supporting Information

S1. Phonon dispersions of $ReNX_4$ and MF_5 nanowires

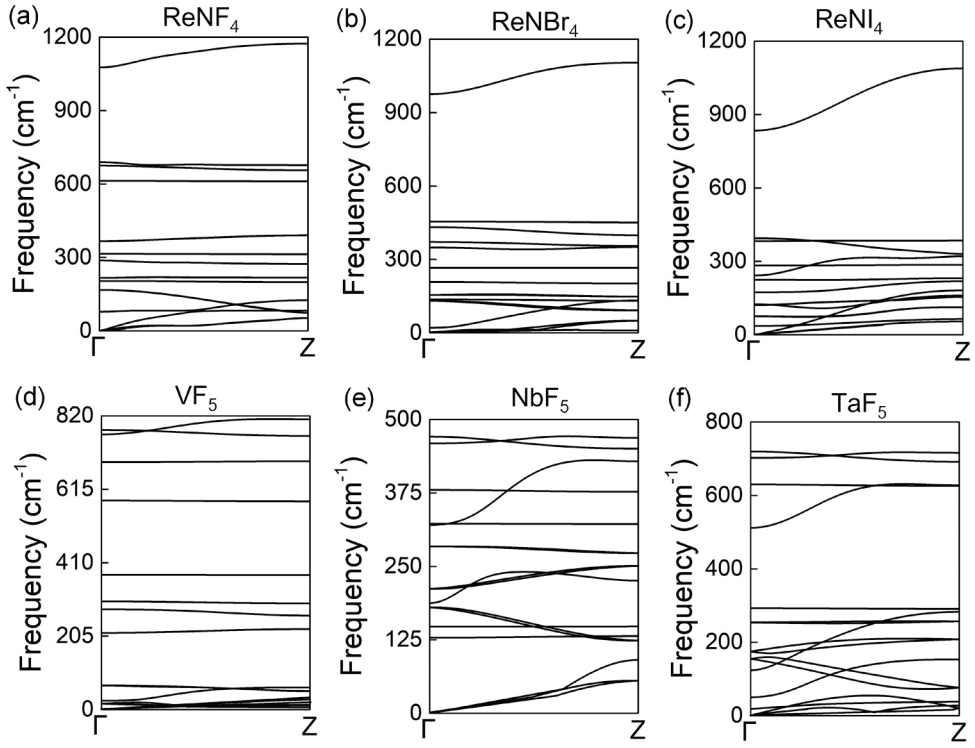

Fig. S1 Phonon dispersion of $ReNX_4$ and MF_5 nanowires.

S2. Band structures of $ReNX_4$ and MF_5 nanowires

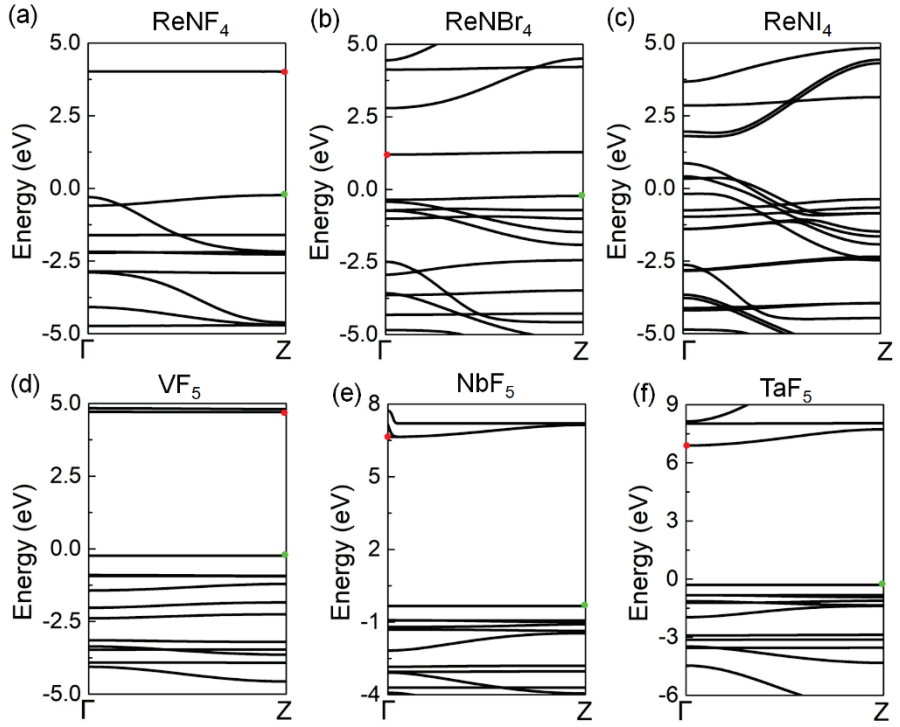

Fig. S2 Band structures of $ReNX_4$ and MF_5 nanowires. The conduction band minimum (CBM) and valence band maximum (VBM) are marked by red and green dots, respectively.

S3. Energy map of $ReNX_4$ and MF_5 nanowires

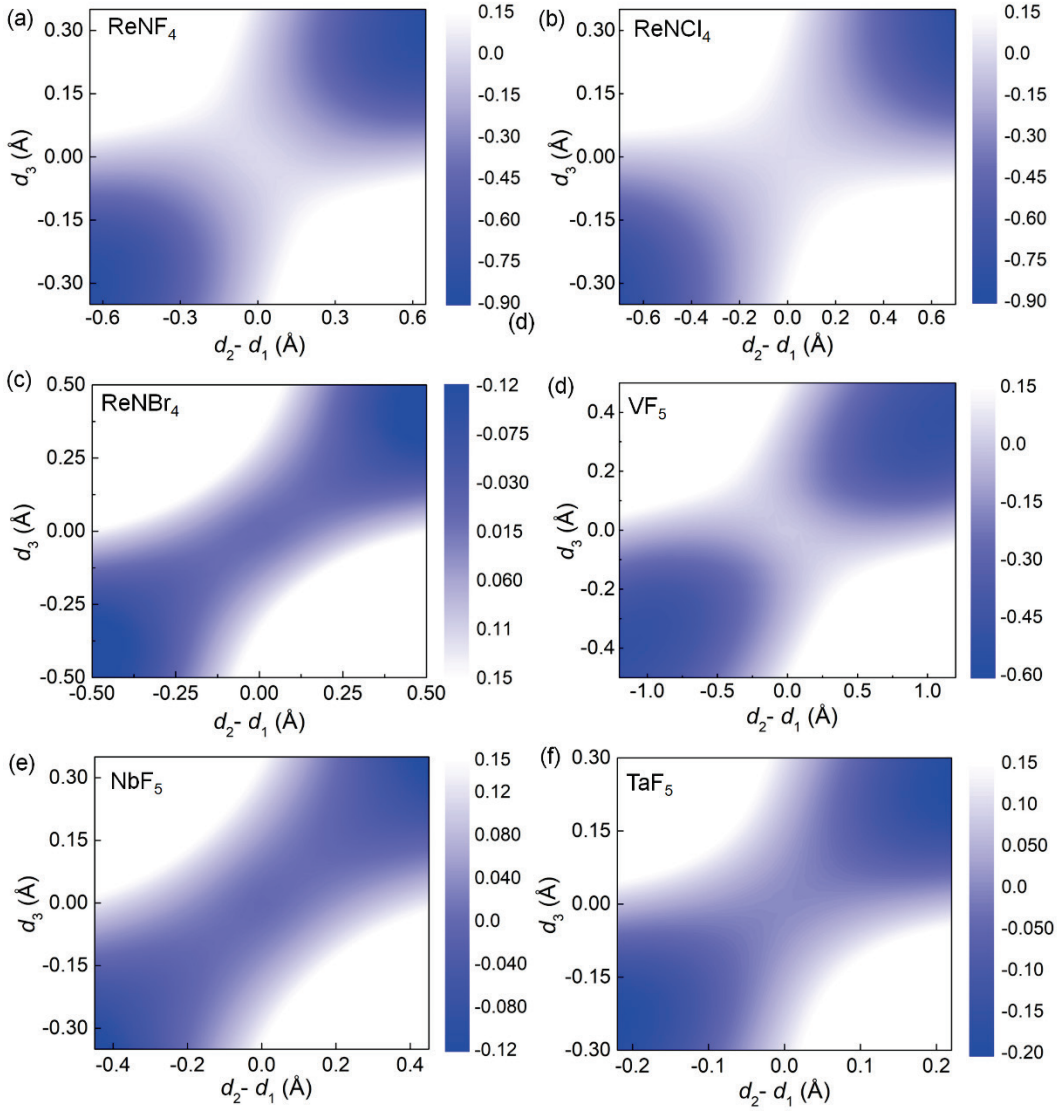

Fig. S3 The energy contour plot (in eV) of 1D $ReNX_4$ and MF_5. The energy of the PE phases is set to zero.

S4. Crystal Orbital Overlap Population (COOP) of $ReNX_4$ and MF_5 nanowires

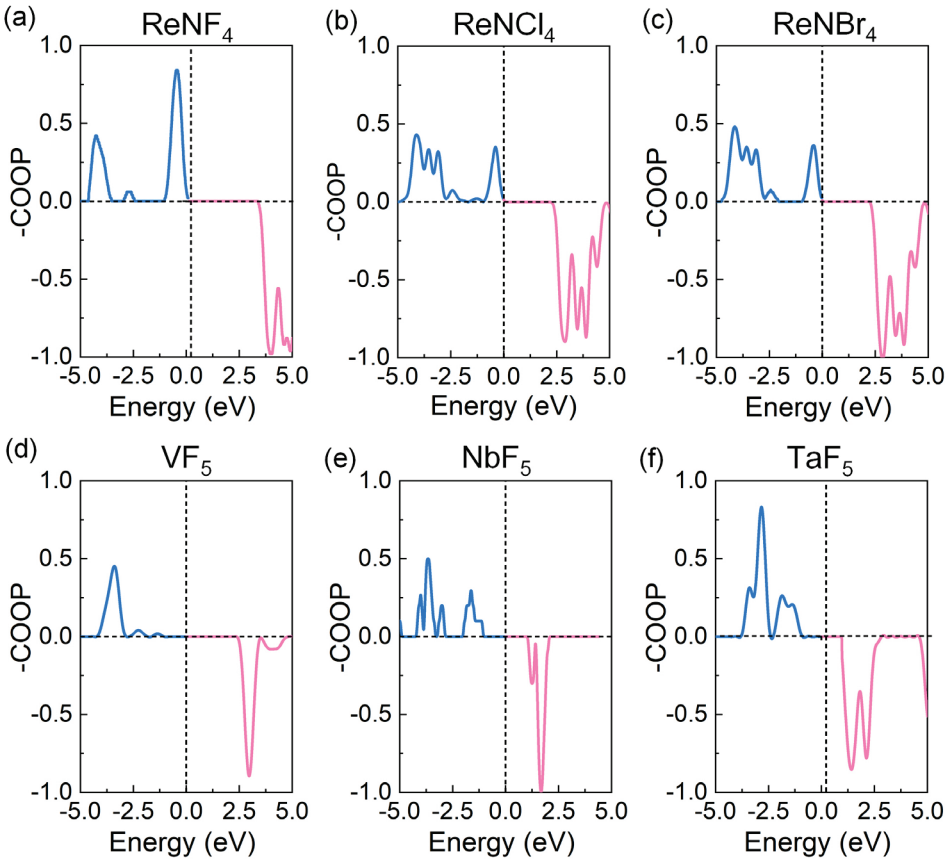

Fig. S4 COOP curves for $ReNX_4$ and MF_5 nanowires.

S5. Double-well potential versus polarization for $ReNX_4$ and MF_5 nanowires

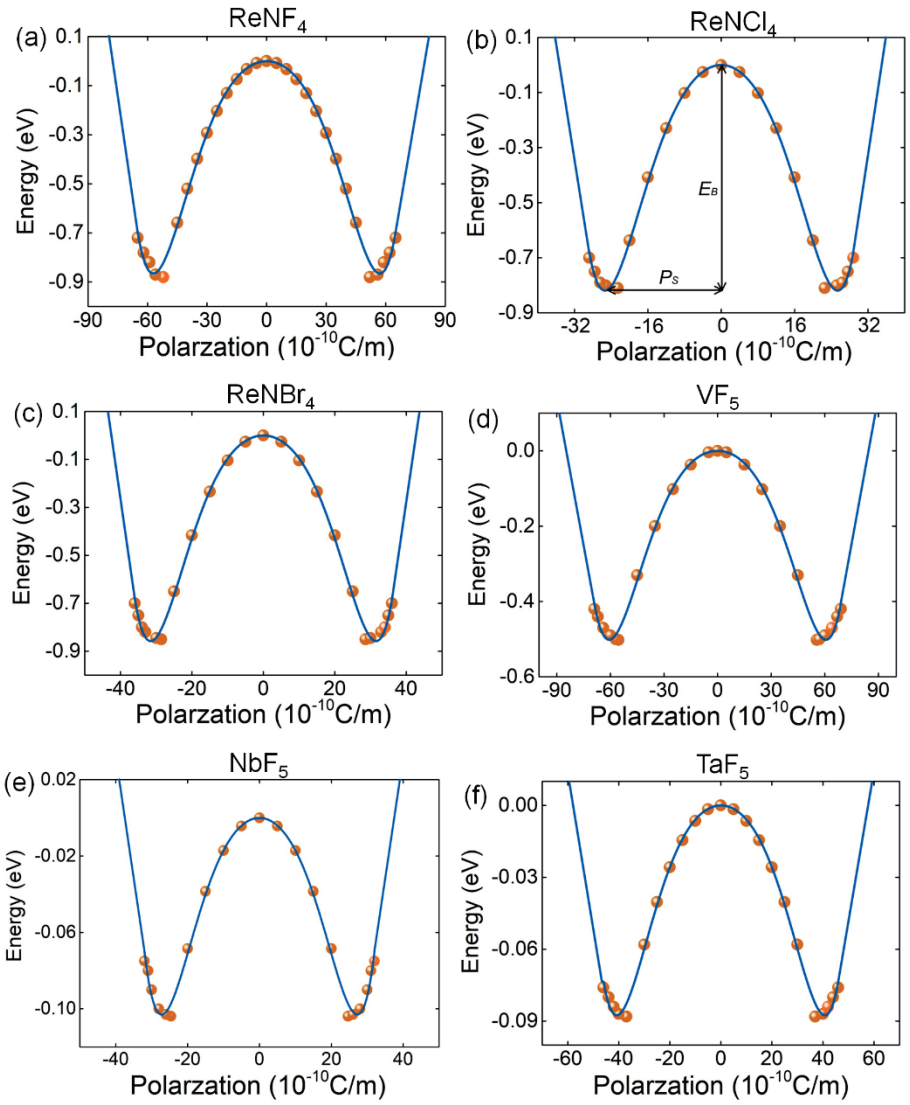

Fig. S5 Double-well potential versus polarization for $ReNX_4$ and MF_5 nanowires.

S6. Dipole-dipole interaction energy for $ReNX_4$ and MF_5 nanowires

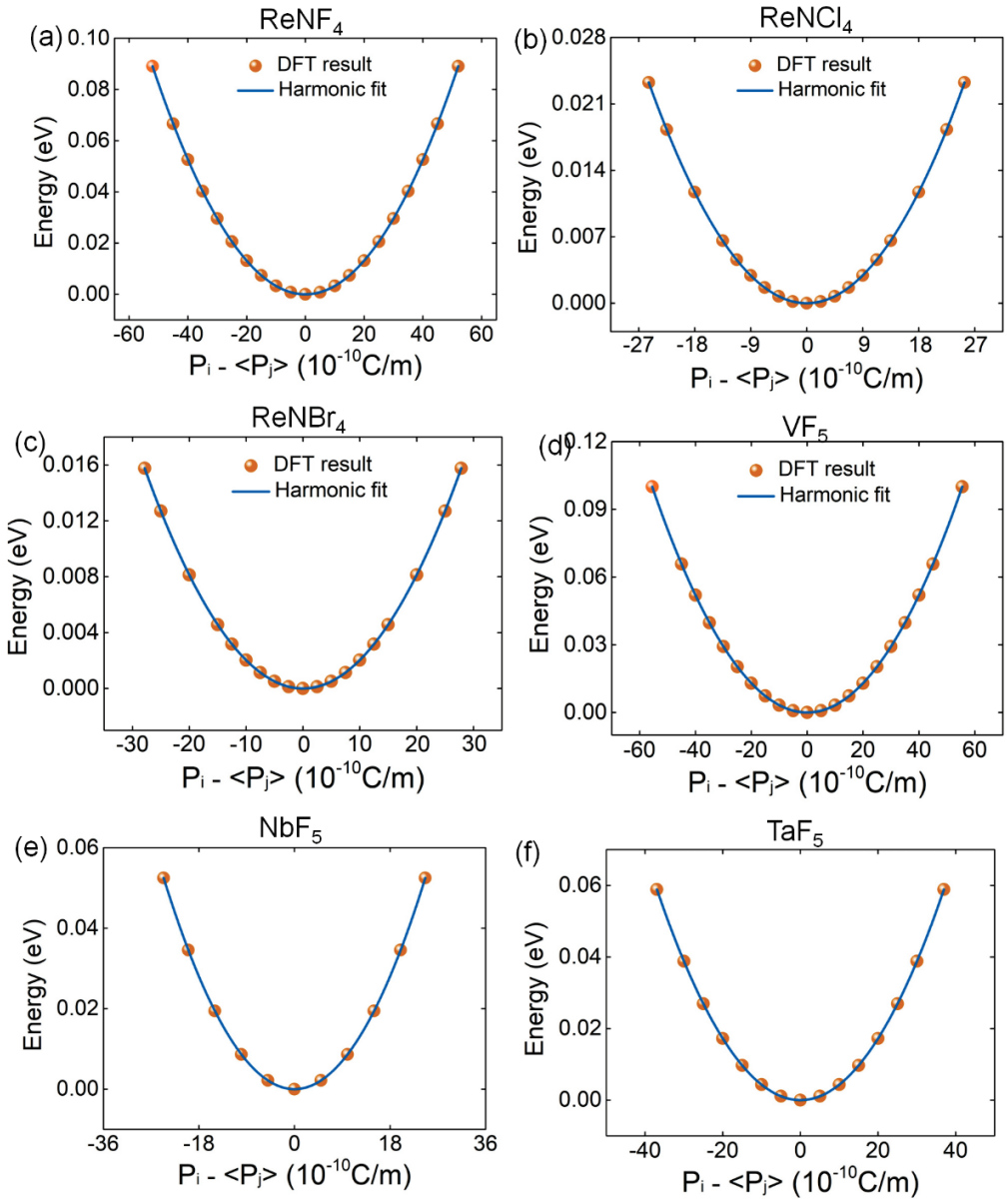

Fig. S6 The dipole-dipole interaction energy for $ReNX_4$ and MF_5 nanowires calculated by using the mean-field method.

S7. Temperature dependence of polarization

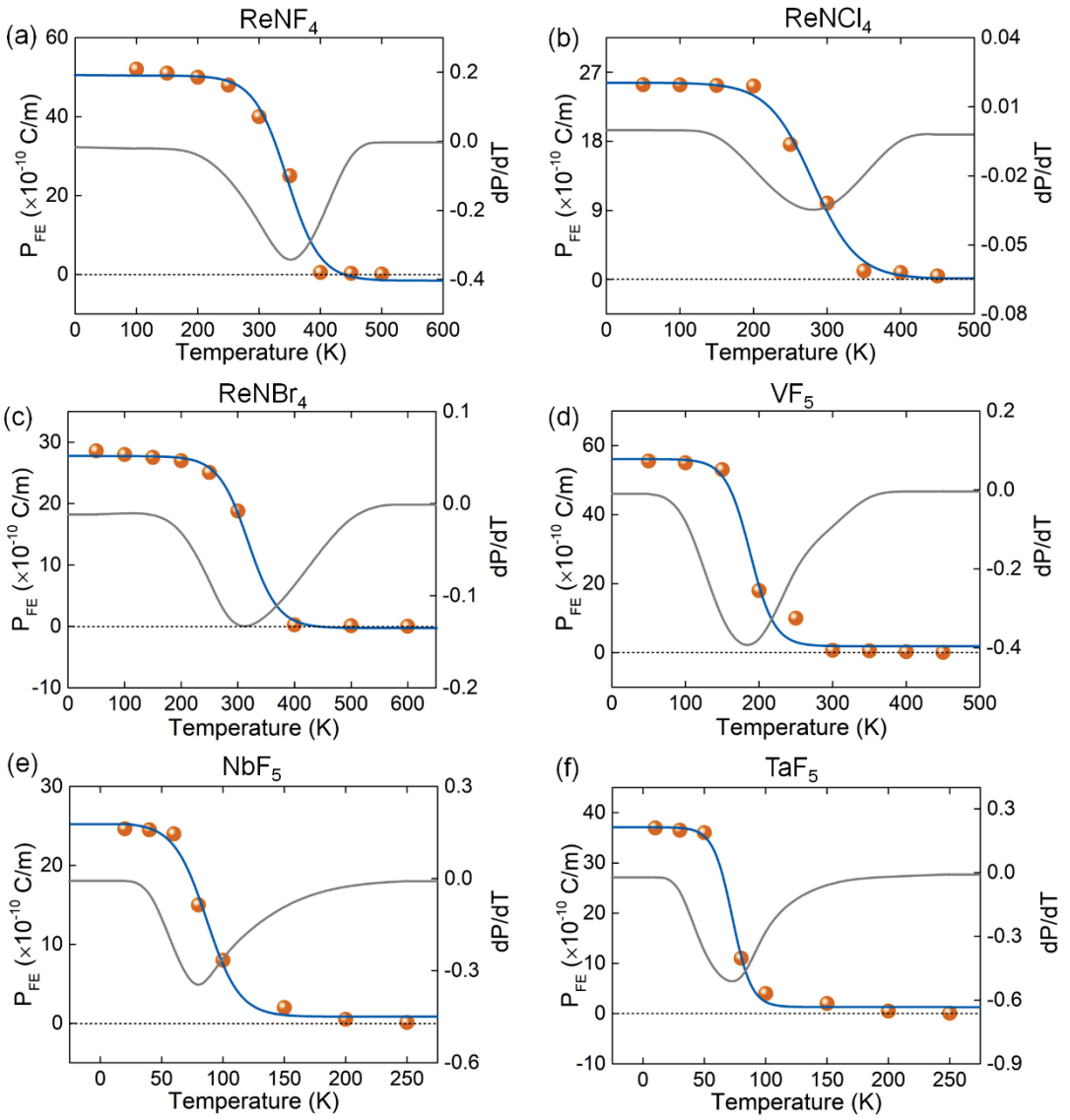

Fig. S7 Temperature dependence of polarization obtained from *ab initio* molecular dynamics (orange balls). Blue line is sigmoid fits to MD results and grey line is the pyroelectric response (dP/dT) for $ReNX_4$ and MF_5 nanowires.

S8. Piezoelectric response for $ReNX_4$ and MF_5 nanowires

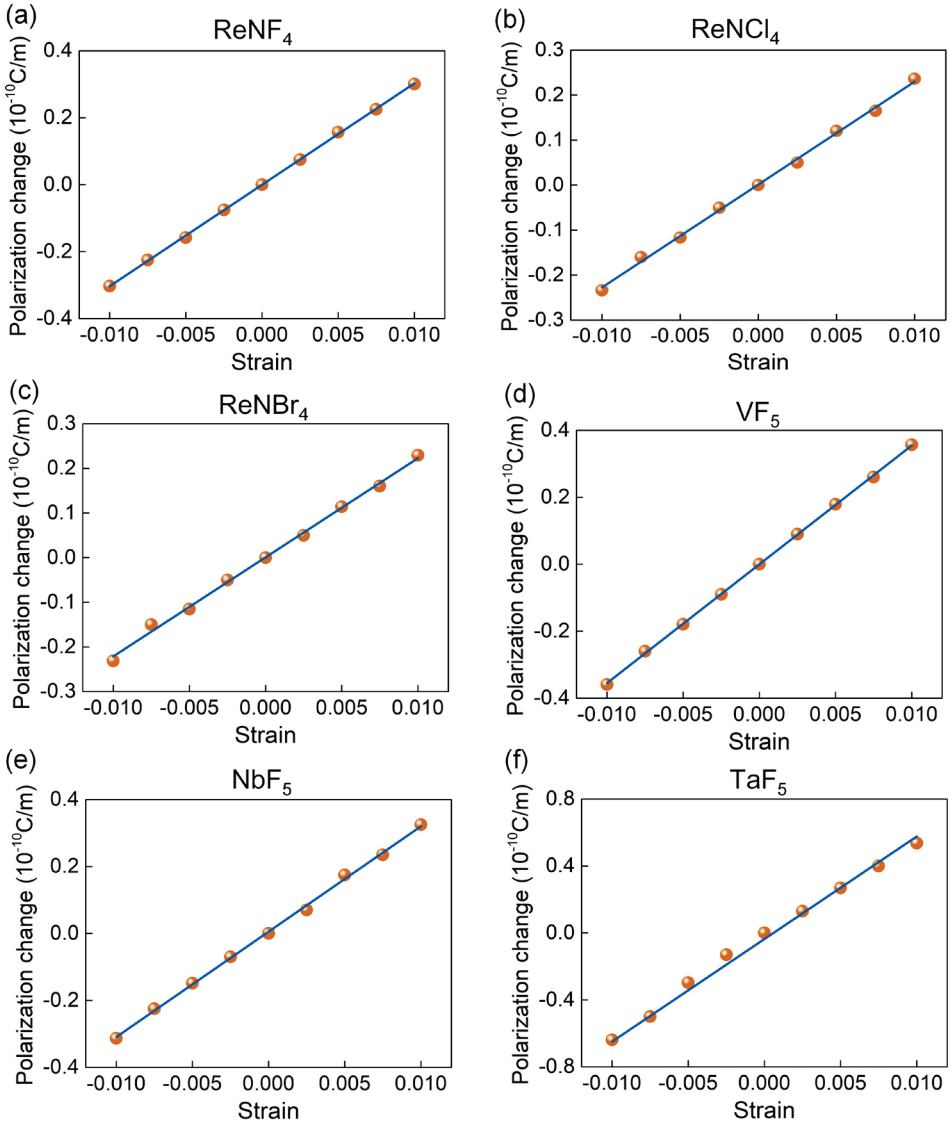

Fig. S8 Piezoelectric response (relaxed-ion e_{11} coefficient) for $ReNX_4$ and MF_5 nanowires from DFT calculation. The polarization and strain are all along *z* direction. The corresponding relaxed-ion piezoelectric coefficient e_{11} can be obtained from the slope of the line.