Supporting Information

Cd_2NF, an analogue of CdO

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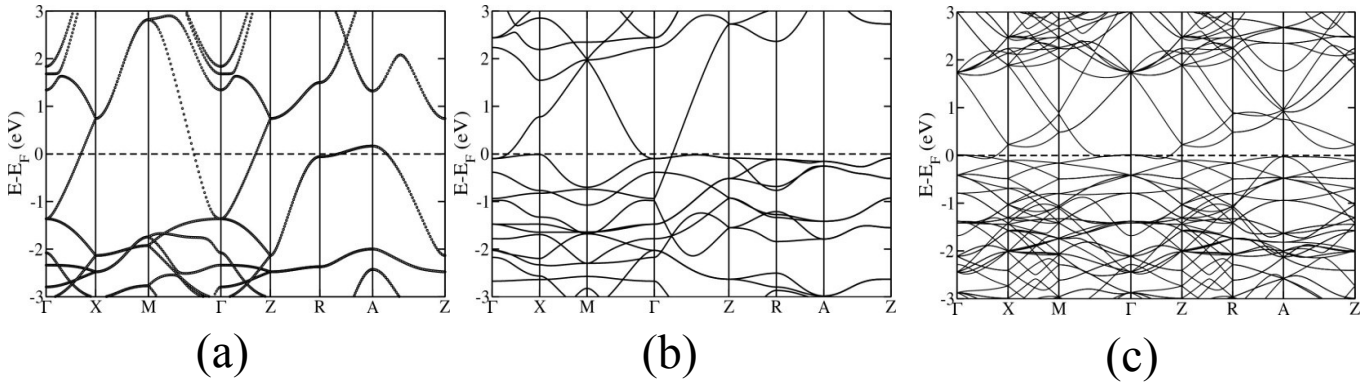
Table S1. Energetics of various ordering of N and F atoms in 1x1x1, √2x√2x√1 (configuration III has been considered here), and 2x2x2 supercell of Cd_2NF obtained using LDA ultrasoft pseudopotential (LDA-USPP) and PAW.

Supercell	**ΔE (eV/u.c.)**	
	LDA-USPP	**PAW**
1x1x1	0.533	0.51
√2x√2x1	0	0
2x2x2	0.530	0.28



FigureS1 Electronic structure of various ordering of N and F atoms in (a) √2x√2x1, and (b) 2x2x2 supercells of Cd_2NF, obtained from calculations based on PAW.

TableS2. Standard deviations of Rietveld-refined lattice parameters and bond lengths.

a=b=c= 4.7052 (±5) Å

Atom	X	Y	Z	Biso	Occ
Cd	0	0	0	0. 245 (±3)	0.47
N	0.488 (±1)	0.488 (±1)	0.488 (±1)	0. 420 (±2)	N=0.382
F	0.488 (±1)	0.488 (±1)	0.488 (±1)	0. 420 (±2)	F=0.218