

# Phase Diagram of Multiferroic $\text{CuFeO}_2$

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Because they offer the ability to control magnetism with electric fields, multiferroic materials have attracted great interest. Recently, ferroelectric coupling has been discovered in several frustrated magnets, where simple collinear (CL) magnetic order with all spins aligned along one axis is not possible due to the lattice topology.

One such class of materials,  $\text{CuFeO}_2$ , becomes multiferroic either with magnetic field or by replacing the magnetic Fe ions with non-magnetic Al or Ga ions.

We have predicted the phase diagram of  $\text{CuFeO}_2$  as a function of magnetic field  $H$  and anisotropy  $D$ , which decreases with Ga or Al doping and

increases with excess of deficient oxygen in the non-stoichiometric compound  $\text{CuFeO}_{2+\delta}$ .  $\text{CuFeO}_2$  was modeled as a two-dimensional triangular lattice with antiferromagnetic exchange coupling  $J_1 < 0$  between neighboring spins.

The predicted phase diagram shown above contains several candidate multiferroic phases where the spin states are non-collinear (NC) (not all spins lie along the same axis) and chiral (there is a special screw axis). In addition to the observed complex non-collinear (CNC) phase, the phase diagram also contains a conical spin-flop (SF) phase and three NC phases (shaded in the phase diagram above) with periods containing 5 atoms. Since the NC and SF phases are chiral, they may also exhibit ferroelectric coupling.

