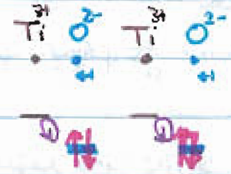
Multiferroics and Magnetoelectrics [Mostovoy]

- The Maxwell Eqns. has duality properties $\begin{Bmatrix} E \\ B \end{Bmatrix} \longleftrightarrow \begin{Bmatrix} B \\ -E \end{Bmatrix}$.

- However, ferromagnets (FM) breaks time-reversal, while ferroelectric (e.g. $BaTiO_3$) (FE) breaks inversion symmetry.

- From quantum chemistry, { FM wants partial d-shell; FE wants empty d-shell }

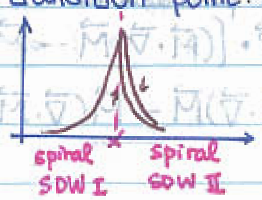
  $\Longrightarrow$ small overlap for multiferroics



- First linear magnetoelectric effect: Cr_2O_3

$$P = \chi_e E + \alpha H, \quad M = \alpha E + \chi_m H.$$

- Around the same time multiferroics is also observed.
  - ▲ In these material, electric polarization changes dramatically around magnetic transition point.
  - ▲ e.g. $DyMnO_3$ (giant magnetocapacitance



- Phenomenlogy of linear magnetoelectric effect

$$P_i = \alpha_{ij} H_j \qquad \Longleftrightarrow \qquad \Phi_{ME} = -\alpha_{ij} E_i H_j$$
$$M_i = \alpha_{ji} E_j$$

These material breaks time-reversal & space-inversal symmetry. But respects the combination of both.

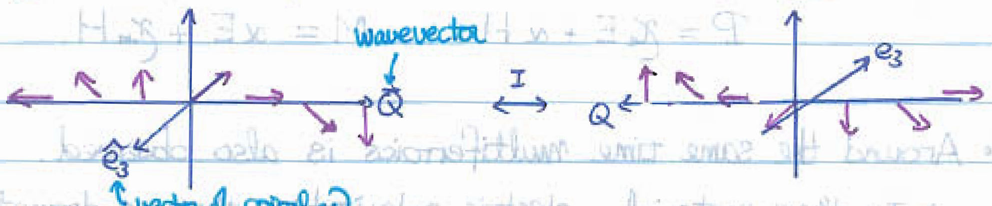
- ▲ Practically, one just need to check that the observed symmetry of a material satisfies the desired symmetry to find magnetoelec candidate.
- ▲ Given symmetry, write down all possible terms respecting the symmetry to obtain a theory.

- More theoretically, one can write down all the Ginzburg–Landau term consistent with symmetry.

- Ferroelectrics

	space-inversion breaking mechanism	materials
proper	covalent bond	$BaTiO_3$
proper	atom polarizability	$BiMnO_3$
improper	(geometric FE) ↓ structural transition	K_2SeO_4
improper	(electronic FE) ↓ charge ordering	$LuFe_2O_4$
improper	(magnetic FE) ↓ magnetic ordering	$CoCr_2O_4$

- Magnetic FE —— spiral SDW breaks inversion



- To describe the induced polarization:

$$F_P = \frac{P^2}{2\chi_e} - \lambda \vec{P} \cdot \left[(\vec{M}\cdot\vec{\nabla})\vec{M} - \vec{M}(\vec{\nabla}\cdot\vec{M}) \right]$$

$$\longrightarrow \vec{P} = \lambda \chi_e \left[(\vec{M}\cdot\vec{\nabla})\vec{M} - \vec{M}(\vec{\nabla}\cdot\vec{M}) \right]$$

- In comparison, sinusoidal SDW has no polarization; while for spiral SDW,

- To get multiferroic, one way is to consider frustration (geometric or by further bonds.

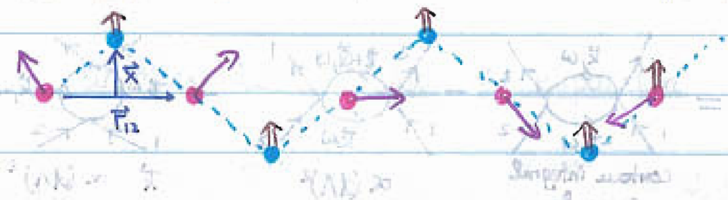
e.g. RMnO$_3$

- $T_{FE} < T_M$ because there is a sinusoidal–helicodial transition

$$\Phi = a_x M_x^2 + a_y M_y^2 + a_z M_z^2 + \frac{b}{2} M^4 + c\vec{M}\left(\frac{\partial^2}{\partial x^2} + Q^2\right)^2 \vec{M}$$

$$\Longrightarrow \vec{M} = M_x \hat{x} \cos(Qx) \quad \longmapsto \quad \vec{M} = M_x \hat{x} \cos(Qx) + M_y \hat{y} \sin(Qx)$$

- Microscopically, Dzyaloshinskii–Moriya causes multiferroic effect



$$\mathcal{E}_{DM} = \vec{D}_{12} \cdot (\vec{S}_1 \times \vec{S}_2)$$
$$\vec{D}_{12} \propto \lambda \vec{x} \times \vec{r}_{12}$$

▲ DM is originated from 1st-order correction to super-exchange by spin-orbit coupling.

- Another microscopic mechanism is magnetostriction.

- A third mechanism is exchange striction

▲ recall $\theta \sim 180° \Rightarrow J\ 0$ & $\theta \sim 90° \Rightarrow J < 0$

- Another mechanism is higher order term in effective spin Hamiltonian from Hubbard model

- Finally, polarization can come from bi-hopping of e^- on O^{2-}