The linear magnetoelectric effect

\[ P_i = \alpha_{ij} H_j \]
\[ M_i = \alpha_{ji} E_j \]

\( \alpha \) is the magnetoelectric tensor

non-zero only in the absence of space- and time-inversion

Design new interfacial magnetoelctrics?

**Tactic:**

- use a ferromagnet (or material with magnetic ordering) to lift time inversion symmetry
- use the interface to lift space inversion symmetry

**Trial system:**

$\text{SrRuO}_3 / \text{SrTiO}_3$ heterostructures

$\text{SrTiO}_3$: insulating perovskite, high permittivity

$\varepsilon_{\text{exp}} \sim 20000$

$\text{SrRuO}_3$: ferromagnetic metallic perovskite; popular electrode for capacitors
Magnetoelectric effects within DFT

Two difficulties:

1) Infinite crystal in uniform external field does not have a ground state:

2) Potential with electric field is non-periodic

Solved using tricks:


M. Stengel and N.A. Spaldin, Ab-initio theory of metal-insulator interfaces in finite electric field, PRB 75, 205121 (2007).
Practical approach to electric fields in DFT for periodic insulators

Minimize electric enthalpy $F$ (instead of Kohn-Sham energy $E_{KS}$)

$$F = E_{KS} - \Omega \cdot \mathbf{P} \cdot \mathbf{E}$$

Express $E_{KS}$ and $\mathbf{P}$ in terms of field-polarized Bloch functions: allows periodic boundary conditions

Discretize k-space: ensures $F$ has minima and prevents Zener charge leakage

How to Obtain $\mathbf{P}$? (next)
Polarization in a pure insulator can be written as a gradient in $k$-space (Berry phase) integrated over filled bands.


For metallic capacitors, we use hermaphrodite Wannier functions (localized in 1D) to obtain polarization.

Magnetoelectric response of interface

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Origin of effect: carrier-mediated magnetoelectricity
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E-field switchable magnetization