The linear magnetoelectric effect

$$P_i = \alpha_{ij} H_j$$

$$M_i = \alpha_{ji} E_j$$

α is the magnetoelectric tensor

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

The revival of the magneto-electric effect, M. Fiebig, J. Phys. D **38**, R123 (2005)

Design new interfacial magnetoelectrics?

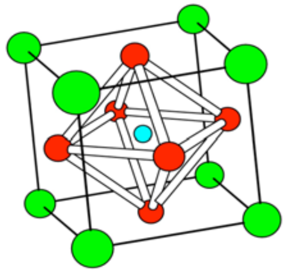
Tactic:

use a ferromagnet (or material with magnetic ordering) to lift time inversion symmetry

use the interface to lift space inversion symmetry

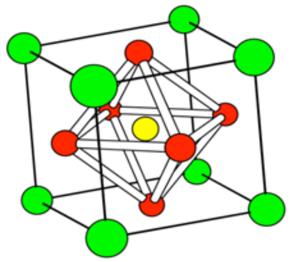
Trial system:

$SrRuO_3$ / $SrTiO_3$ heterostructures



$SrTiO_3$: insulating perovskite, high permittivity

ε_{exp} ~ 20000

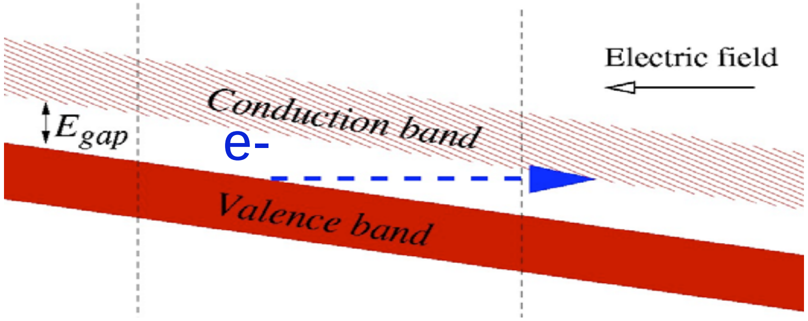


$SrRuO_3$: ferromagnetic metallic perovskite; popular electrode for capacitors

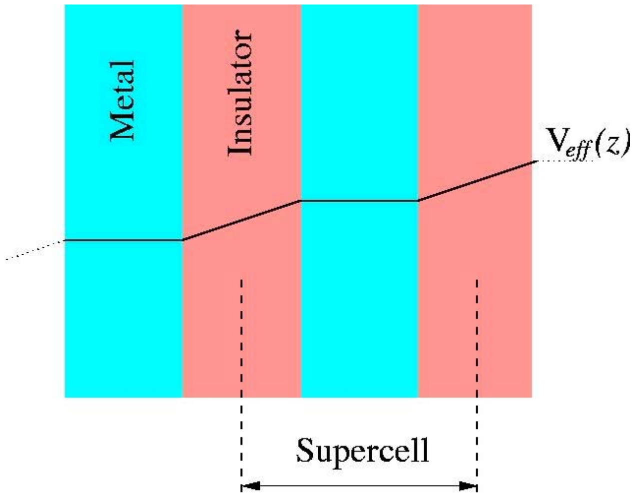
Magnetoelectric effects within DFT

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:

I. Souza, J. Iniguez and D. Vanderbilt, *First-principles approach to insulators in finite electric fields*, Phys. Rev. Lett. **89**, 117602 (2002)

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

I. Souza, J. Iniguez and D. Vanderbilt, *First-principles approach to insulators in finite electric fields*, Phys. Rev. Lett. **89**, 117602 (2002)

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

$$F = E_{KS} - \Omega \, P . \mathcal{E}$$

Express E_{KS} and 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 P? (next)

Calculation of P

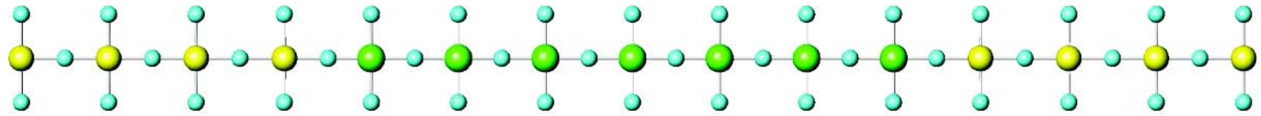
Polarization in a **pure insulator** can be written as a gradient in ***k*-space** (Berry phase) integrated over filled bands

R. D. King-Smith and D. Vanderbilt, *Theory of polarization of crystalline solids*, PRB **47**, 1651 (1993)

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

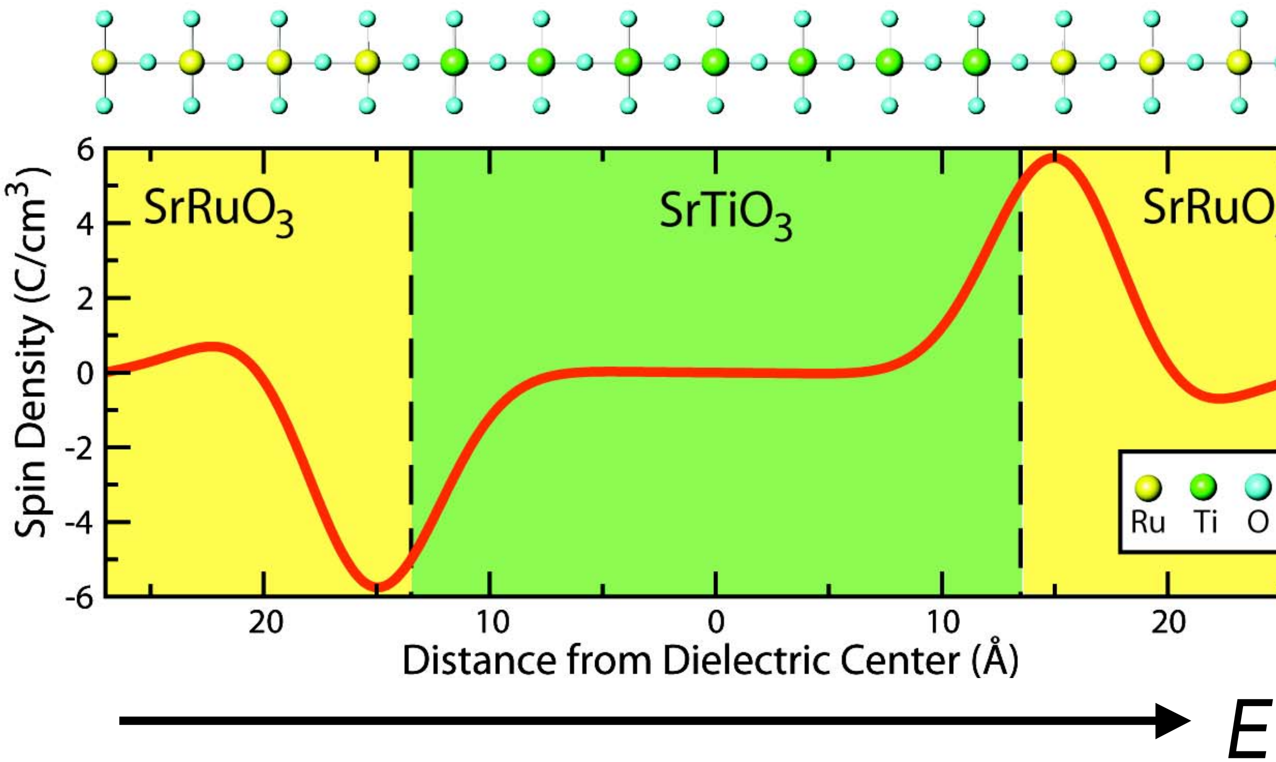
M. Stengel and N. Spaldin, *Ab-initio theory of metal-insulator interfaces in finite electric field,* PRB **75**, 205121 (2007).

Magnetoelectric response of interface



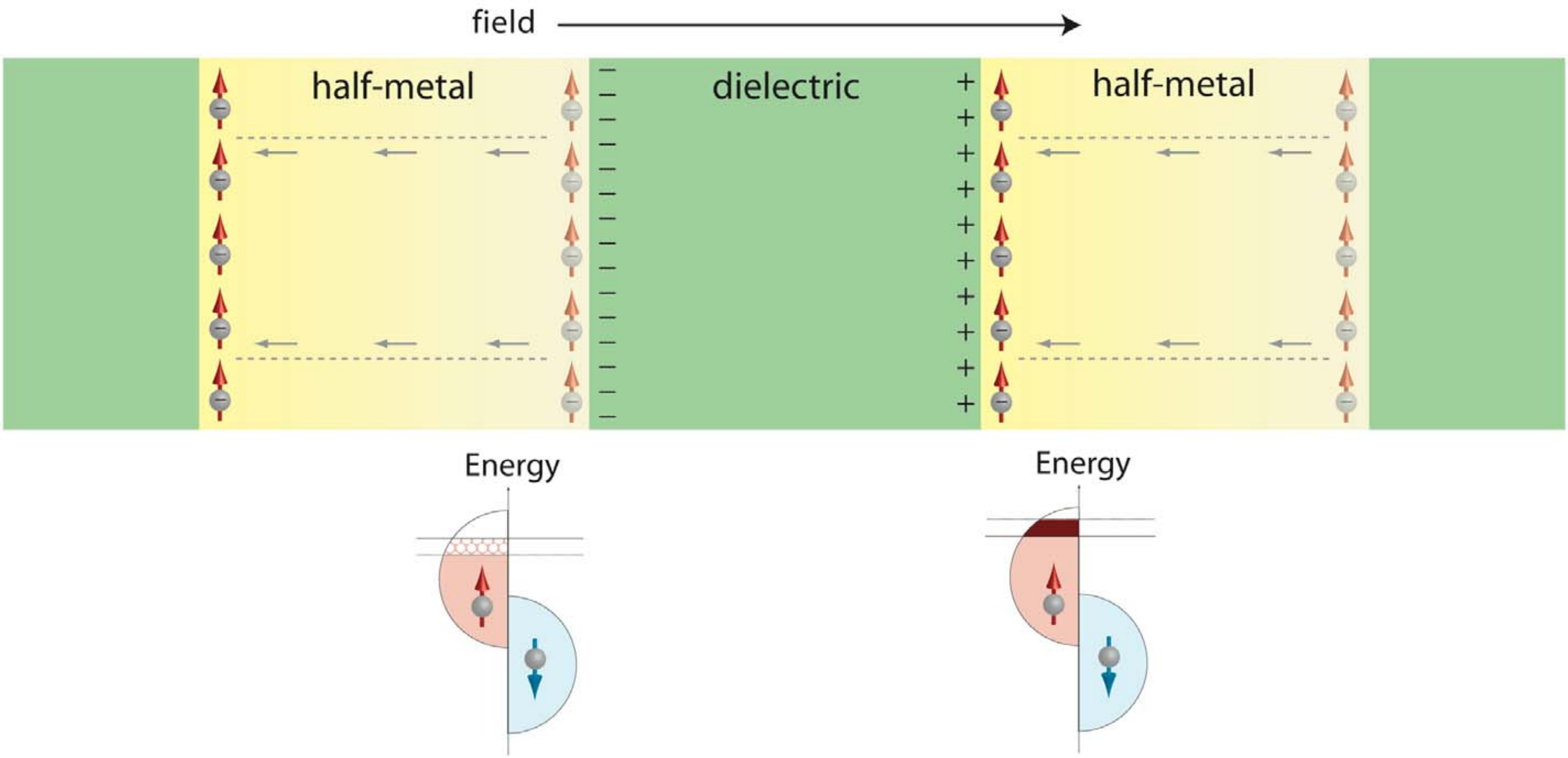
J.M. Rondinelli, M. Stengel and N.A. Spaldin, *Carrier-mediated magnetoelectricity in complex oxide heterostructures*, cond-mat 0706.2199

Magnetoelectric response of interface

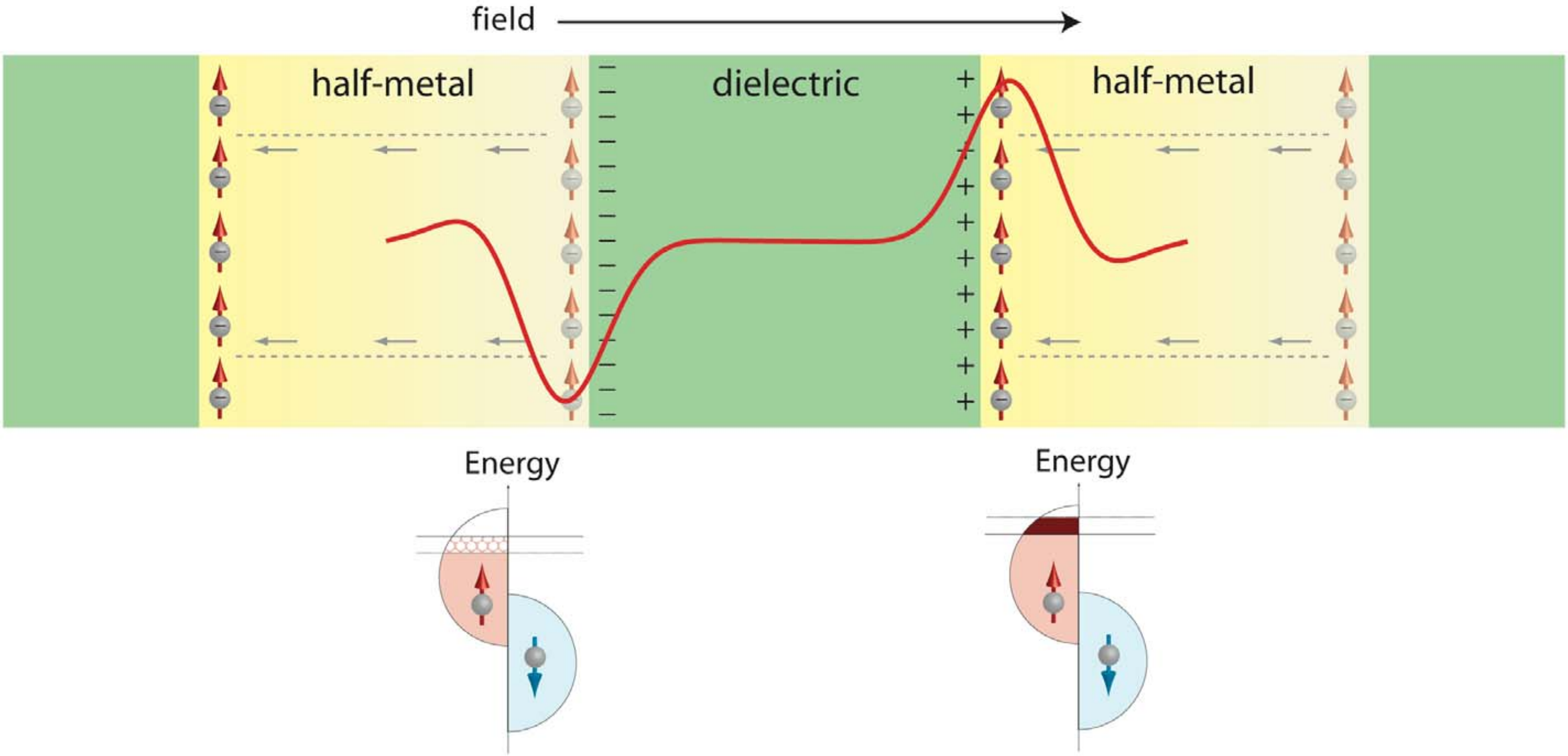


J.M. Rondinelli, M. Stengel and N.A. Spaldin, *Carrier-mediated magnetoelectricity in complex oxide heterostructures*, cond-mat 0706.2199

Origin of effect: carrier-mediated magnetoelectricity



Origin of effect: carrier-mediated magnetoelectricity



E-field switchable magnetization