Computational Nanoferronics Laboratory

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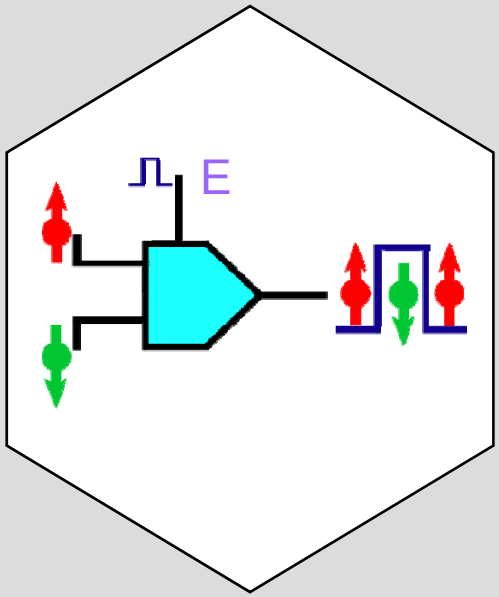
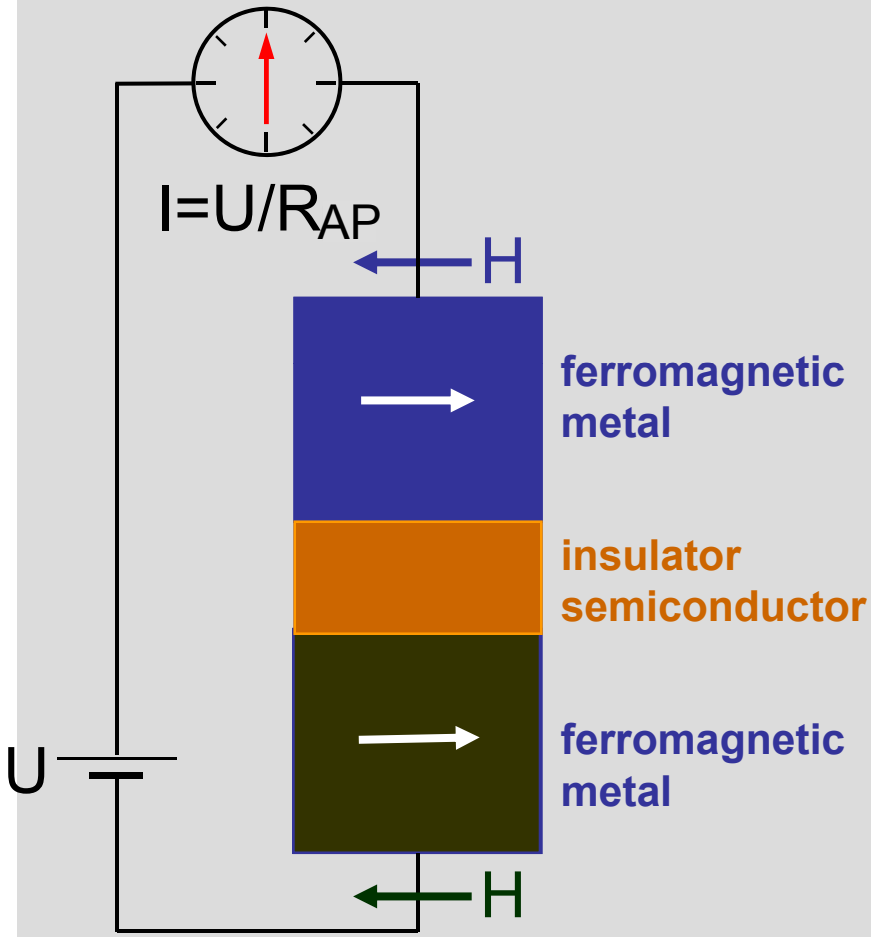
Nanoferronics

Aim: Translate information stored in a ferromagnetic or ferroelectric state into an electric signal

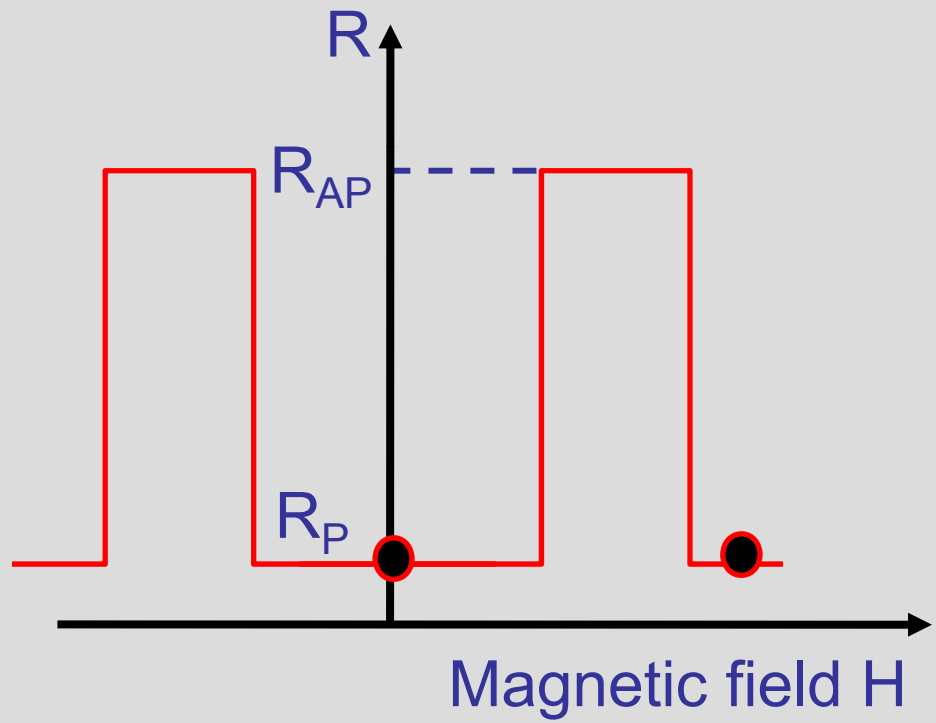


Means: Novel multifunctional materials

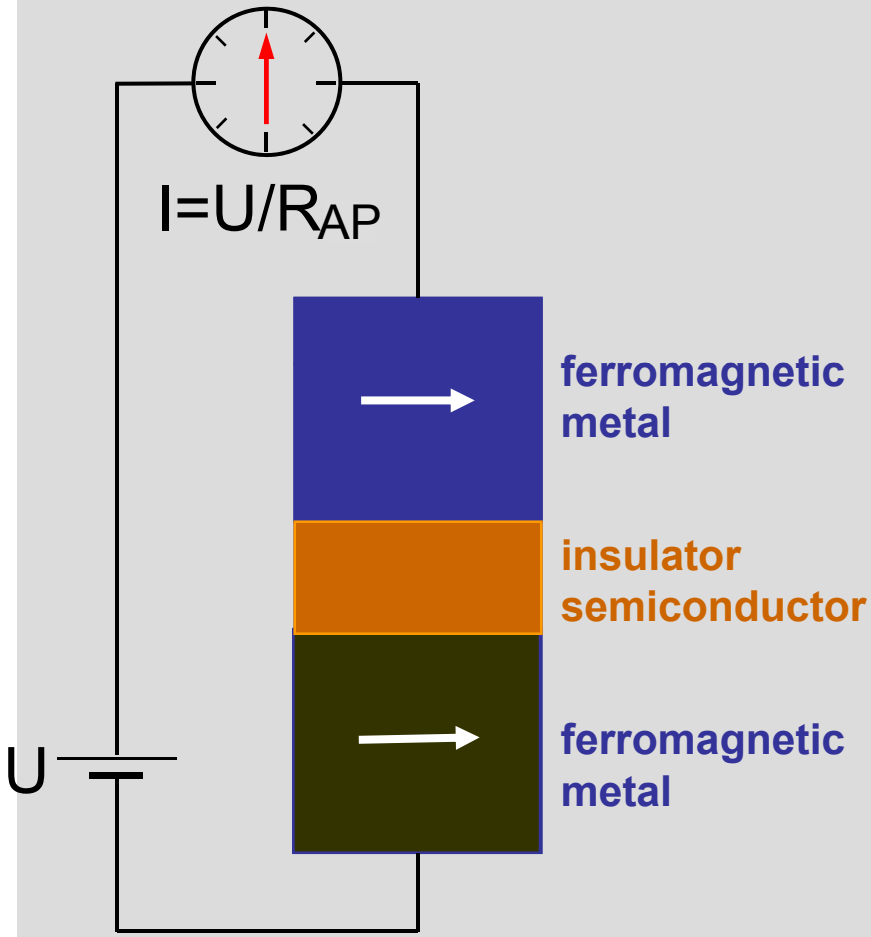
Magnetic tunnel junctions



$$TMR = \frac{R_{AP} - R_P}{R_P}$$



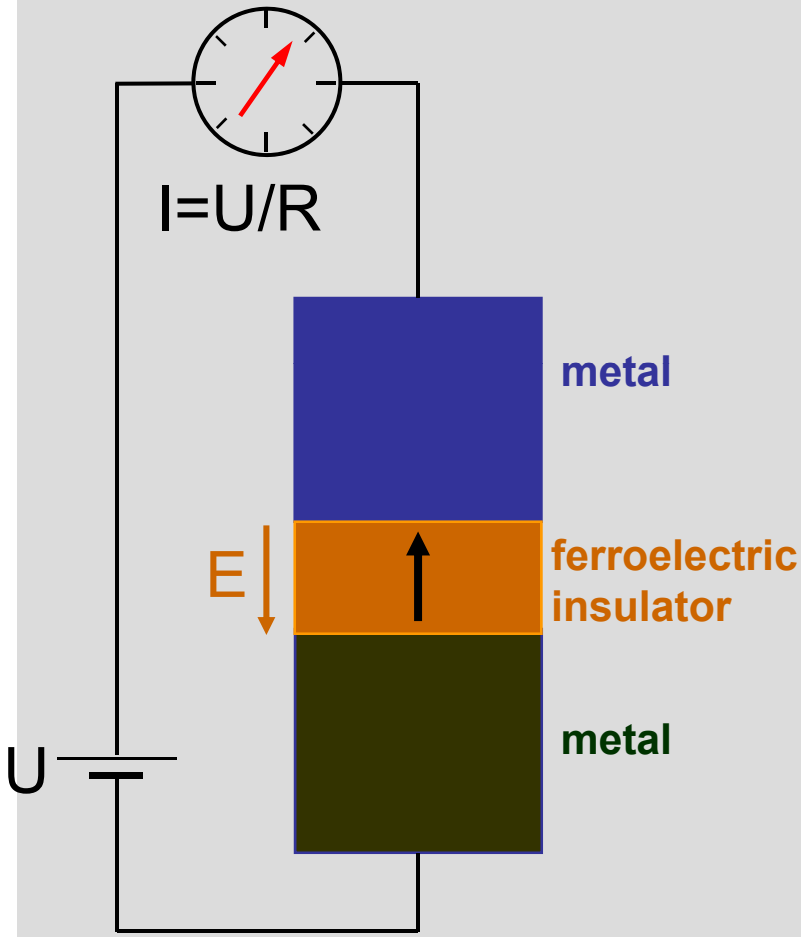
Magnetic tunnel junctions



Magnetic Random Access Memory (MRAM)

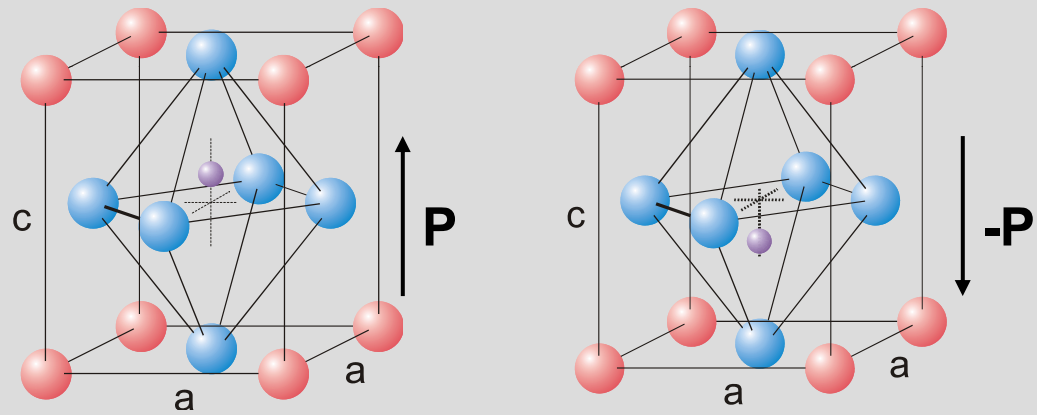
- nonvolatile memory
- low power consumption
- high integration density

Ferroelectric tunnel junctions



Ferroelectric material:

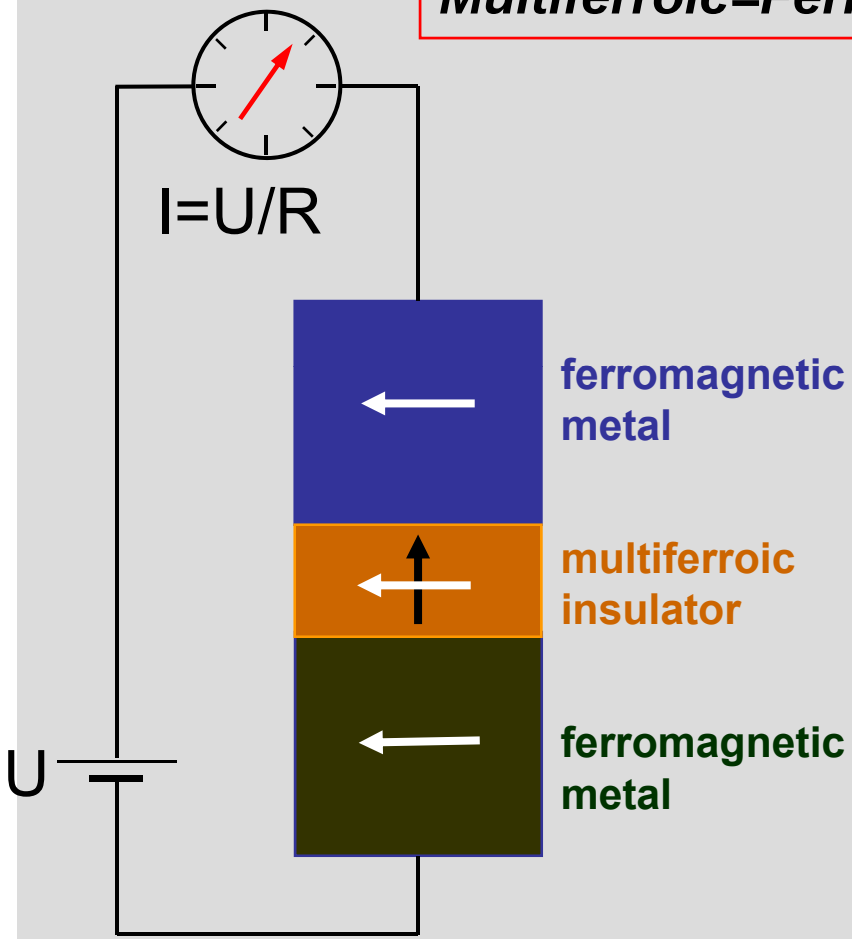
- Spontaneous electric polarization
- Switchable hysteretically by electric field

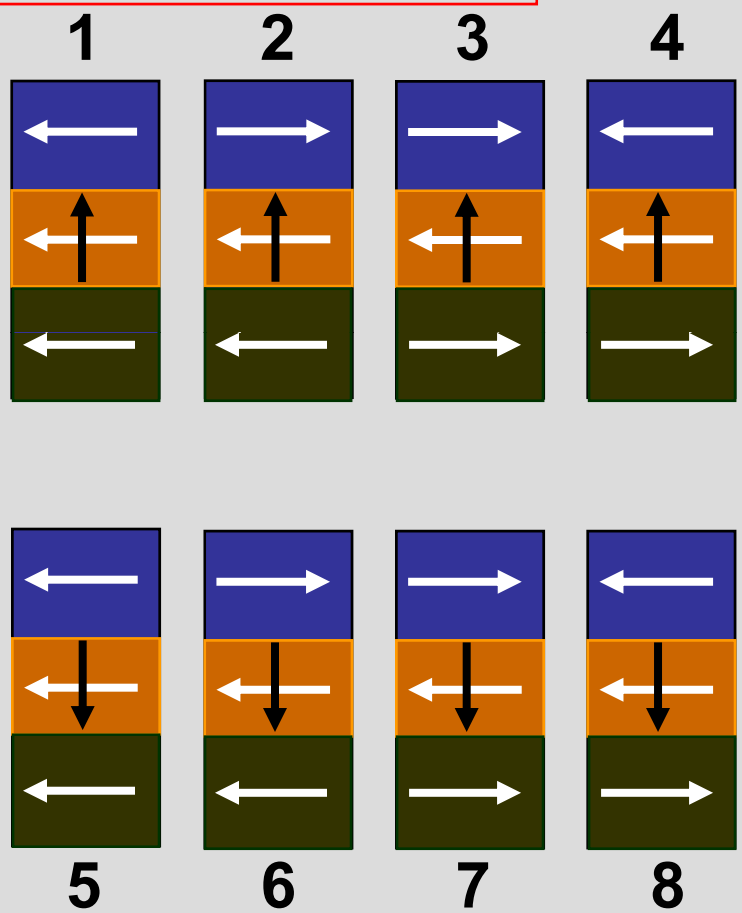


FeRAM

Multiferroic tunnel junctions

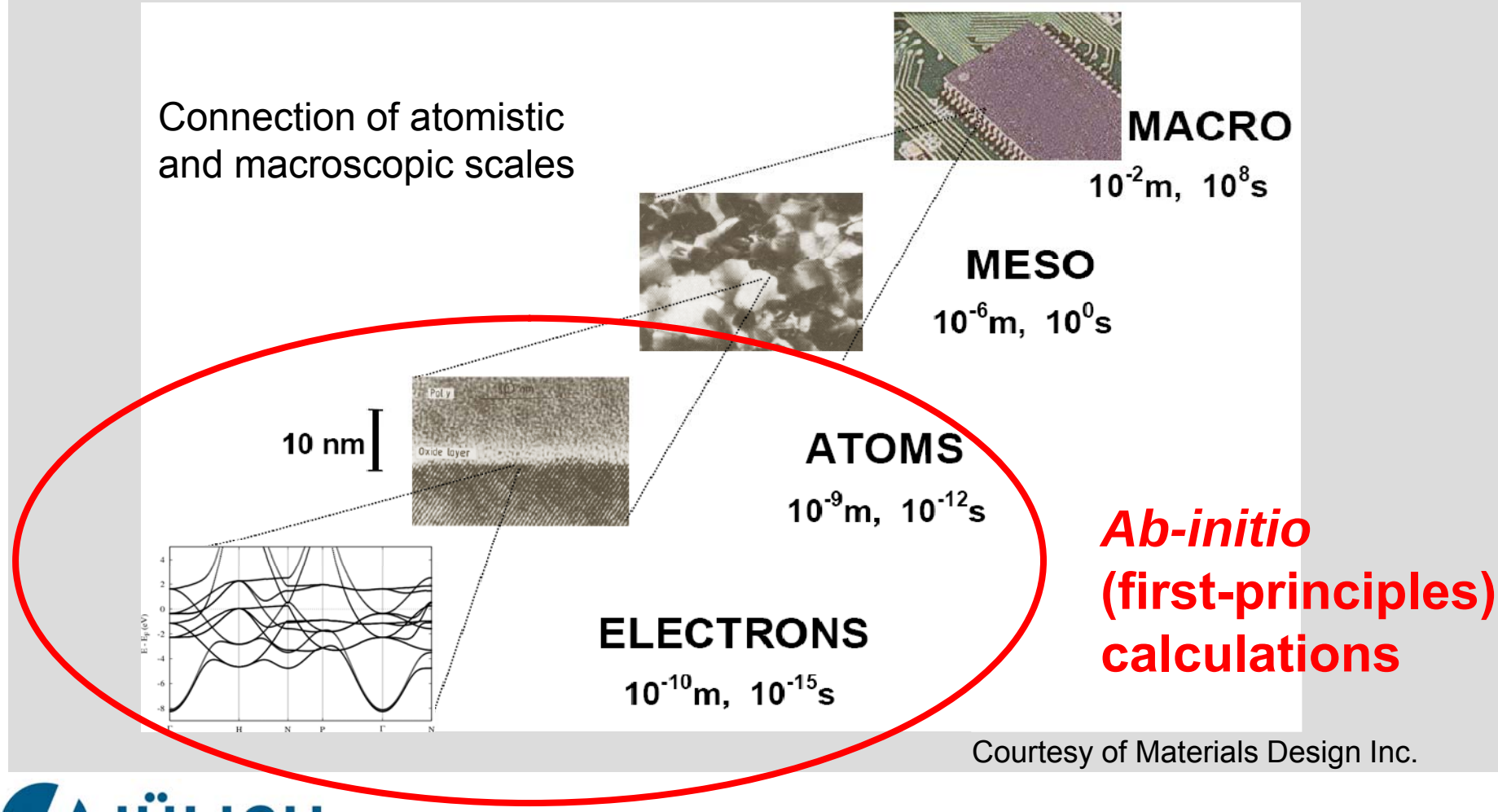
Multiferroic=Ferroelectric+Ferromagnet





Eight different resistive states: **8-bit memory**

The size of the task



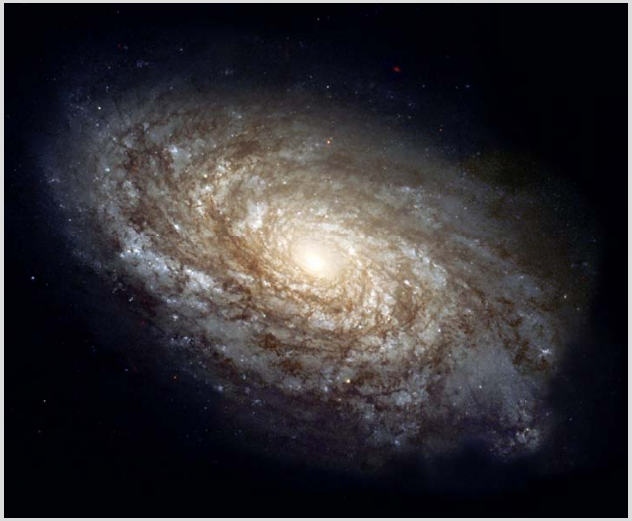
Courtesy of Materials Design Inc.

Quantum Mechanics of Electrons

$$H = -\frac{\hbar^2}{2m}\sum_{j=1}^{N_e}\nabla_j^2 - \sum_{\alpha=1}^{N_i}\frac{\hbar^2}{2M_\alpha}\nabla_\alpha^2 - \sum_{j}^{N_e}\sum_{\alpha=1}^{N_i}\frac{Z_\alpha e^2}{|r_j - R_\alpha|} + \sum_{j<k}^{N_e}\frac{e^2}{|r_j - r_k|} + \sum_{\alpha<\beta}^{N_i}\frac{Z_\alpha Z_\beta e^2}{|R_\alpha - R_\beta|}$$

Schrödinger & Dirac (1929)

- Basic equations are known
- But unsolvable many-body problem



Example: 1 iron atom

26 electron wave-function: $\Psi(r_1,\ldots r_{26})$

store only 10 values per coordinate: 10^{78} values

assume each value could be stored

in a single H atom: **memory heavier than the milky way**

Density Functional Theory

Total Energy:

$$E[\{\mathbf{R}\},\{\hat{\mathbf{M}}\},S,n] = E_{\mathrm{kin}}[n] + E_{\mathrm{H}}[n] + E_{\mathrm{xc}}[n] + E_{\mathrm{ext}}[\{\mathbf{R}\},\{\hat{\mathbf{M}}\},S,n]$$

Secular Equation:

$$\hat{H}[n]\,\psi_i[n] = \varepsilon_i[n]\,\psi_i[n]$$

Density:

$$n(\mathbf{r}) = \sum_{i(occ)}^{M} |\,\psi_i(\mathbf{r})\,|^2$$

Force:

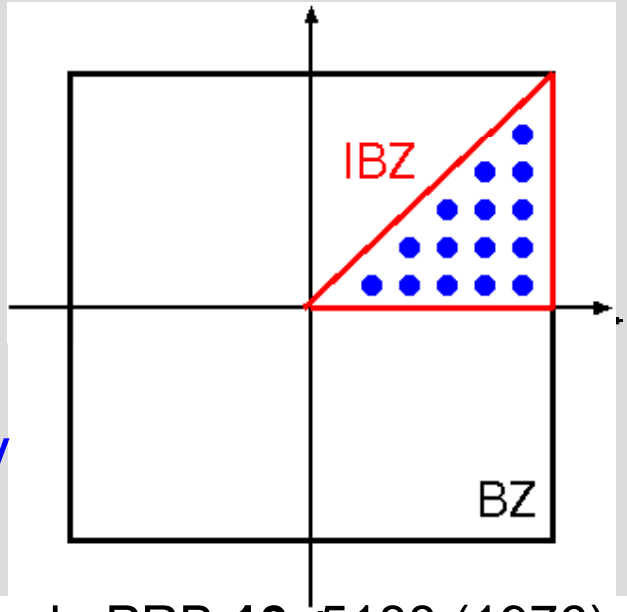
$$\mathbf{F} = -\frac{\partial}{\partial \mathbf{R}}(E[\{\mathbf{R}\},n] + E_{\text{ion-ion}}[\{\mathbf{R}\}])$$

The Planewave Basis

Bloch theorem for periodic solid:

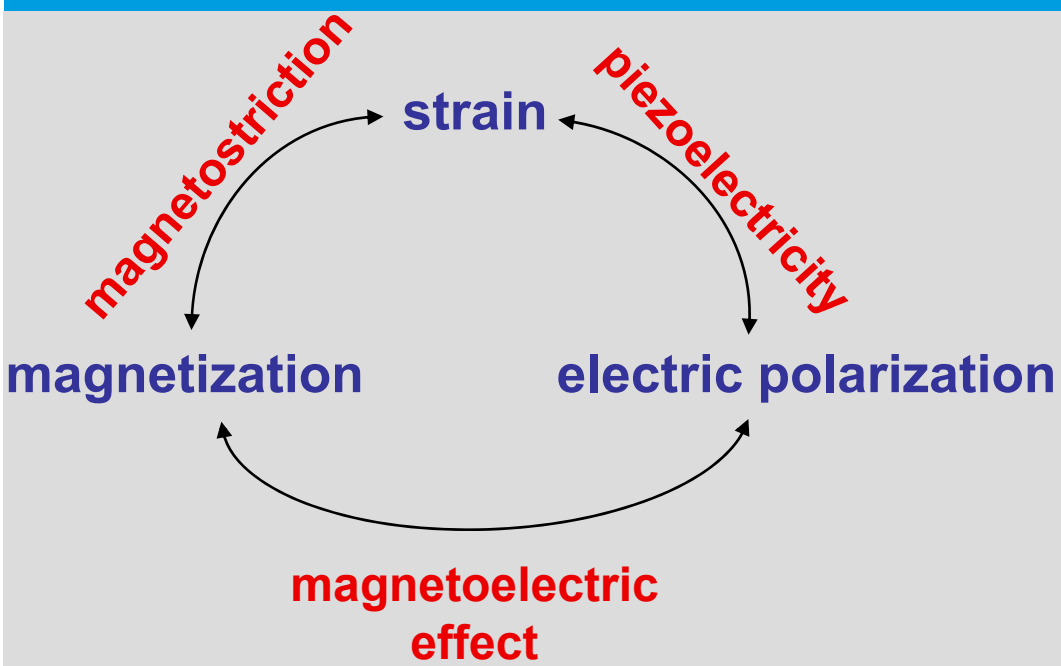
$$\psi_{\mathbf{k},\nu}(\mathbf{r}) = \sum_{|\mathbf{k}+\mathbf{G}|\leq K_{\max}} c^{\mathbf{G}}_{\mathbf{k},\nu} \exp[i(\mathbf{k}+\mathbf{G})\mathbf{r}] \qquad \forall \mathbf{k} \in \mathrm{BZ}$$

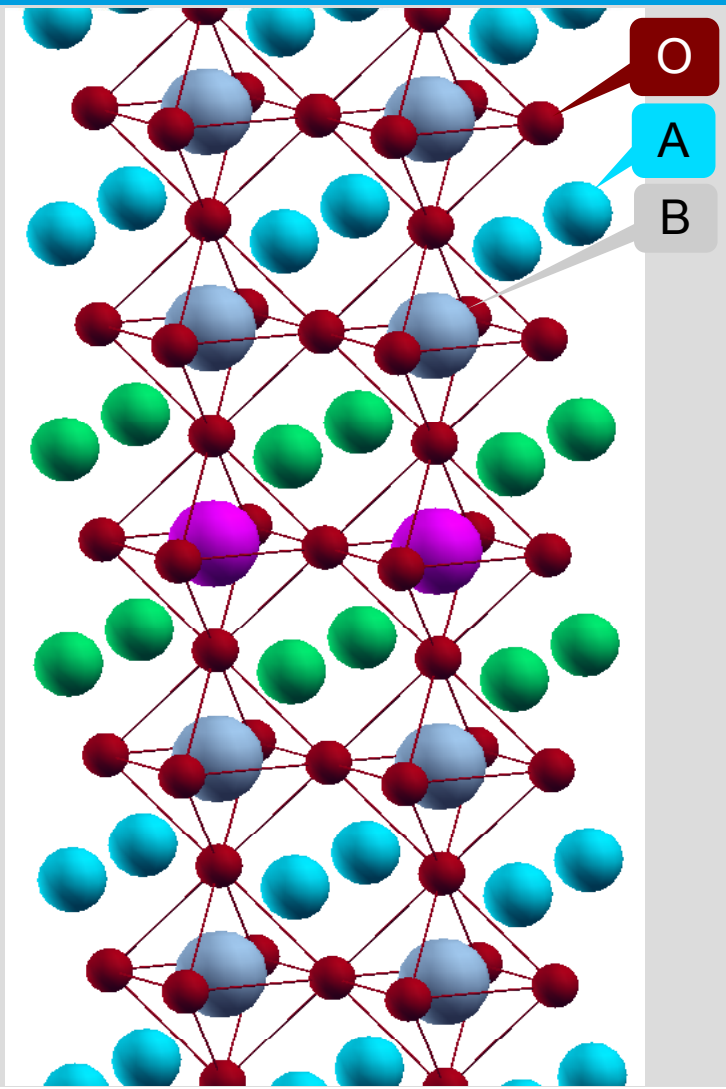
Use point symmetry



H.J. Monkhorst, J.D. Pack, PRB **13**, 5188 (1976)

Perovskites (ABO_3)





Atoms at the interface move to the new equilibrium positions: change in electric & magnetic polarization

Thermal properties from the DFT

Heisenberg Model

$$E = -\tfrac{1}{2}\sum_{i,j} J_{ij}\,\vec{M}_i \cdot \vec{M}_j$$

Calculate J_{ij} within DFT

Possibilities for calculation of J_{ij} :

1. **Lichtenstein's formula (KKR Green function method)**

$$J_{ij} = \tfrac{1}{4\pi}\,\mathrm{Im}\int^{E_F} \mathrm{Tr}\left[G_{ij}^{\uparrow}\Delta t_j G_{ji}^{\downarrow}\Delta t_i\right] dE$$

2. **Frozen magnons, $J(q)$, and Brillouin Zone integration (FLAPW method)**

exchange interaction:

T_C can be calculated within:

- **Mean-field theory**

$$k_B T_C = \tfrac{1}{3}\sum J_{ij} M^2$$

- **Random Phase Approximation**

$$(k_B T_C)^{-1} = 3\sum (J_{ij} M^2)^{-1}$$

- **Monte-Carlo method%**

Jülich – München code
http://olymp.cup.uni-muenchen.de/ak/ebert/SPR-TBKKR

FLEUR code
http://www.flapw.de

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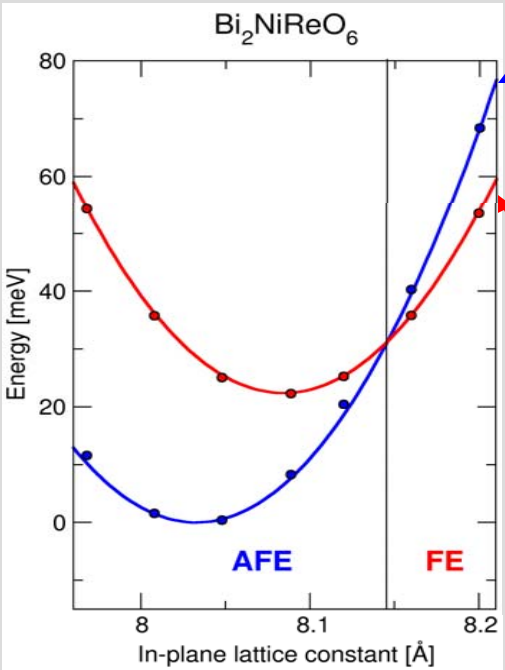
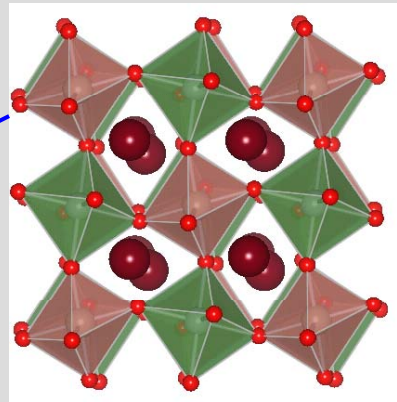
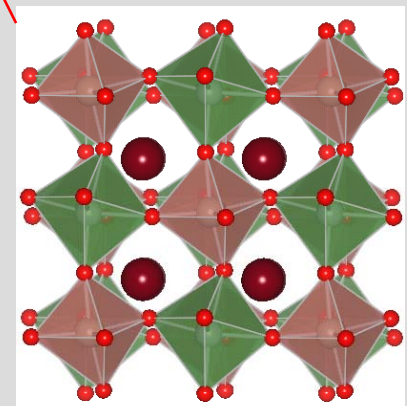
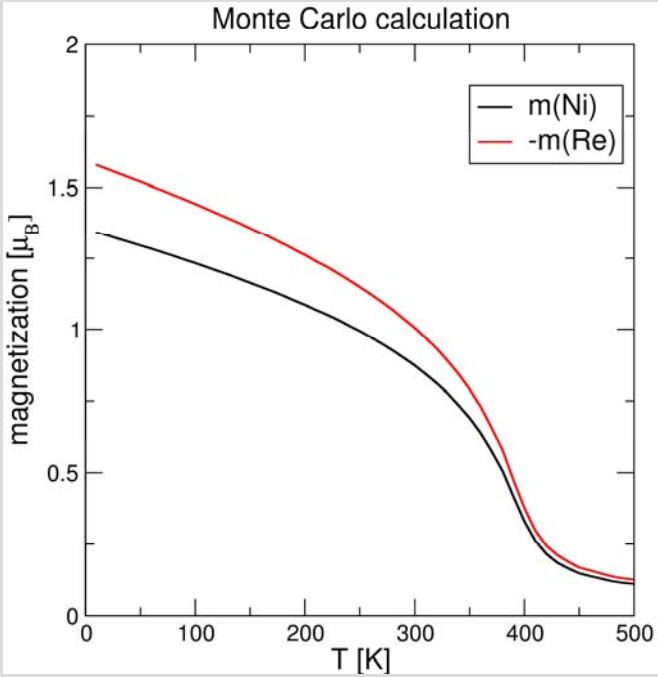
Example: Bi_2NiReO_6

Ground state, symmetry $P\bar{1}$, can be switched to a ferroelectric one with strain









Possible room-temperature multiferroic

Summary & Outlook

- DFT can describe ground state properties of perovskites, giving a satisfactory answer to some questions, but can also be very unreliable for others (e.g. the value of the gap).

- Efficient algorithm for the structural optimization is needed

Thank you!

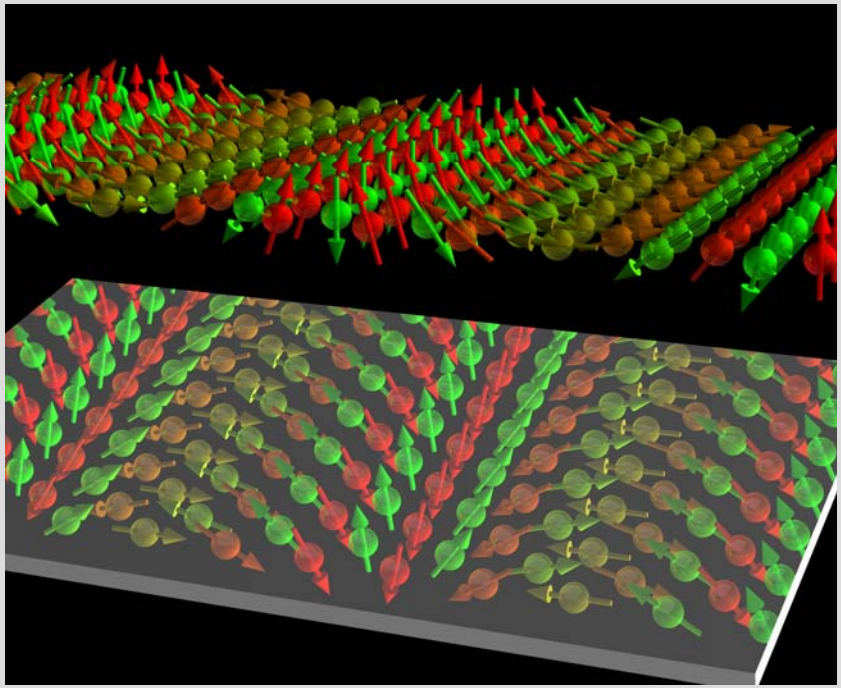
Thank you!

Fleur code

Fleur-code
http://www.flapw.de

FLEUR:

- FLAPW-Method
- LSDA, GGA, LDA+U
- Spin-Orbit Interaction
- 3D-bulk, 2D-Film, 1D-wire
- Total energy + Force
- Spin-polarized
- Non-collinear
- Massively parallelized



*M. Bode et al., Nature **447**, 190 (2007)*
Courtesy P. Ferriani

$$\{H - \varepsilon_\nu S\} c_\nu^G = 0$$

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Basis sets and Eigenvalue Problem

To solve Kohn-Sham equation $\hat{H}\psi = \varepsilon\psi$

➔ introduce basis functions: χ^n

$$\psi_i = \sum_n c_i^n \chi^n$$

$$\sum_n c_i^n \hat{H}\chi^n = \varepsilon_i \sum_n c_i^n \chi^n$$

$$\sum_n \langle \chi^{n'} | \hat{H} | \chi^n \rangle c_i^n = \varepsilon_i \sum_n \langle \chi^{n'} | \chi^n \rangle c_i^n$$

$$\sum_n (H^{n',n} - \varepsilon_i S^{n',n}) c_i^n = 0$$

CPU ≈ N^3_{dim}
≈ N^3_{atom}
≈ V^3, P^3

Density Functional Theory

"**The** Computational Approach with predictive power" **Walter Kohn**

in : Physics, Chemistry, Nanoscience, Materials Science, …

- $\min_{n} E[\{\mathbf{R}\}, \{\hat{\mathbf{M}}\}, S, a|n]$ → Electronic structure, Quantum transport

Total Energy: $E[\{\mathbf{R}\}, \{\hat{\mathbf{M}}\}, S, a|n]$

- $\min_{\{\mathbf{R}\}} E[\{\mathbf{R}\}, \{\hat{\mathbf{M}}\}, S, a|n]$ → Molecular dynamics, Structure determination

- $\min_{\{\hat{\mathbf{M}}\}} E[\{\mathbf{R}\}, \{\hat{\mathbf{M}}\}, S, a|n]$ → Spindynamics, Magnetic structures

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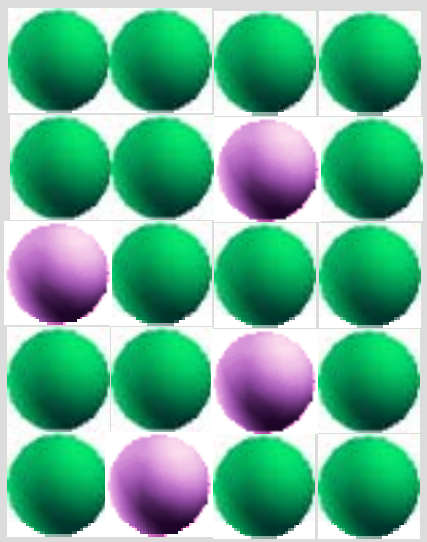
KKR Green-function method

No periodic supercell needed!

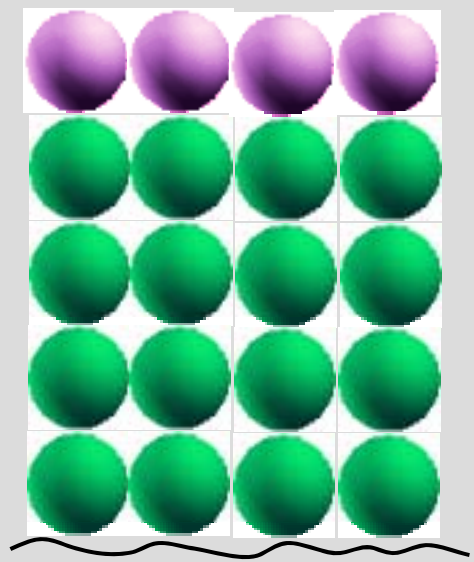
$$G = G_0 + G_0 V G$$

Can treat:

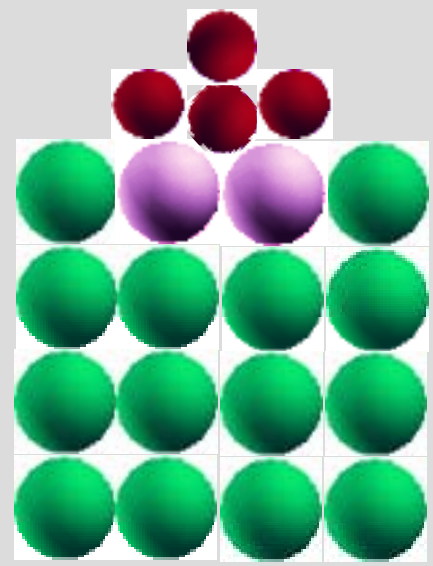
random alloys



semi-infinite crystals



clusters on surfaces



Vision : Nanoferronics

quantum

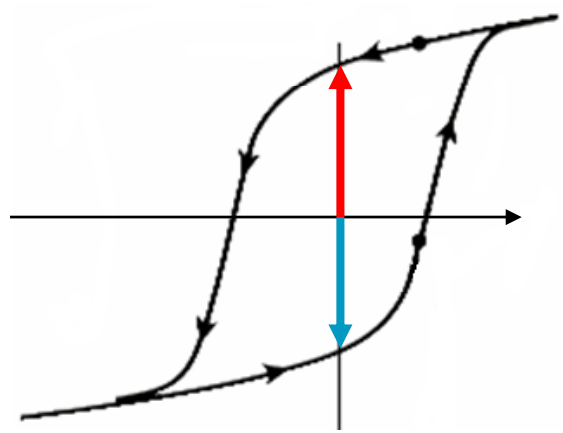
Final Aim:
prediction of new
multifunctional devices

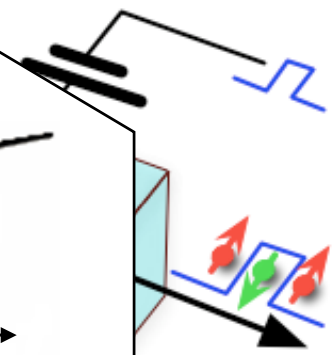
Prof. R. Waser (FZJ)

Prof. U. Klemradt (R
Prof. K. Urban (FZ

Güntherodt (RWTH)
I. Schneider (FZJ)

Hysteresis





fast

Competence in spin… …s and materials design

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