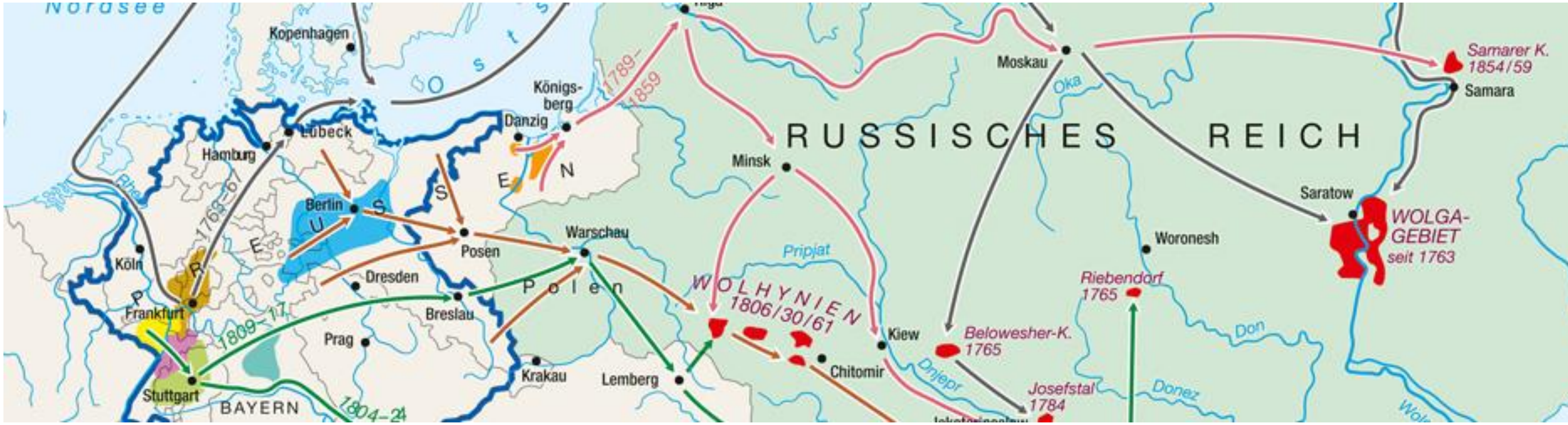
Virtuelles Labor: Forschung und Entwicklung am Computer

Arthur Ernst
Institut für Theoretische Physik

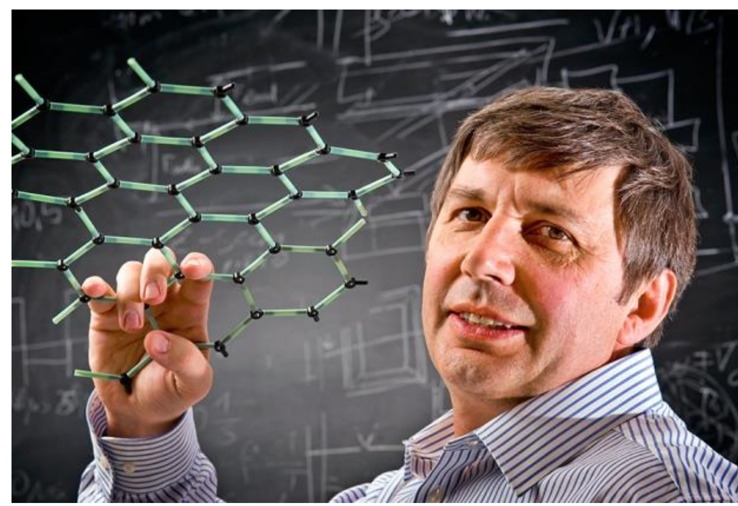
JOHANNES KEPLER
UNIVERSITÄT LINZ

Russia Germans

Russia Germans



Helene Fischer



Andre Geim (Nobel Prize 2010)

Karatau (Kazakhstan)

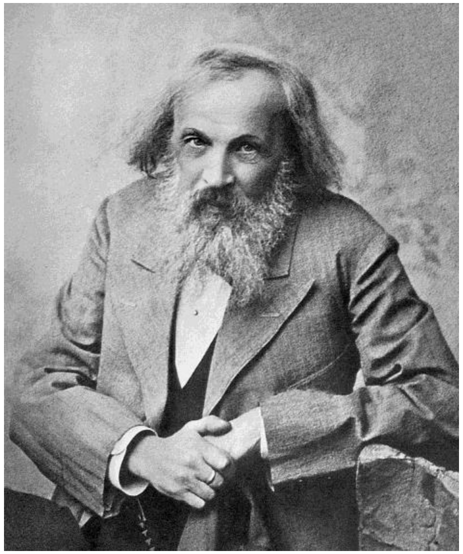
Karatau (Kazakhstan)

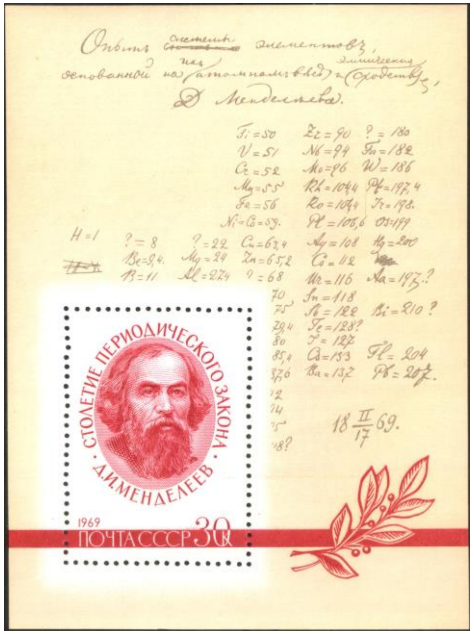
320 sunny days per year
Summer: +10° - +50° C
Winter: -40°- +25° C

Tomsk

6 months winter -50° - 20 °C

University of Tomsk (1985-1993)





Periodic table

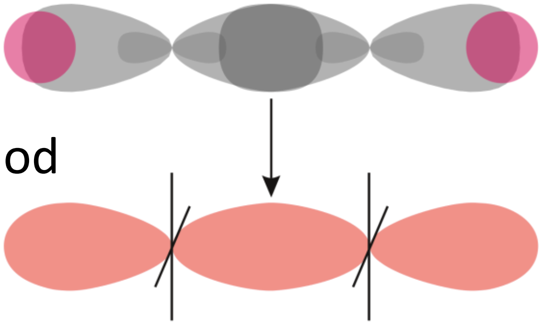
Founded by D. M. Mendeleev in 1878

Dresden (1993-1996)

Helmut Eschrig

Wilhelm Macke

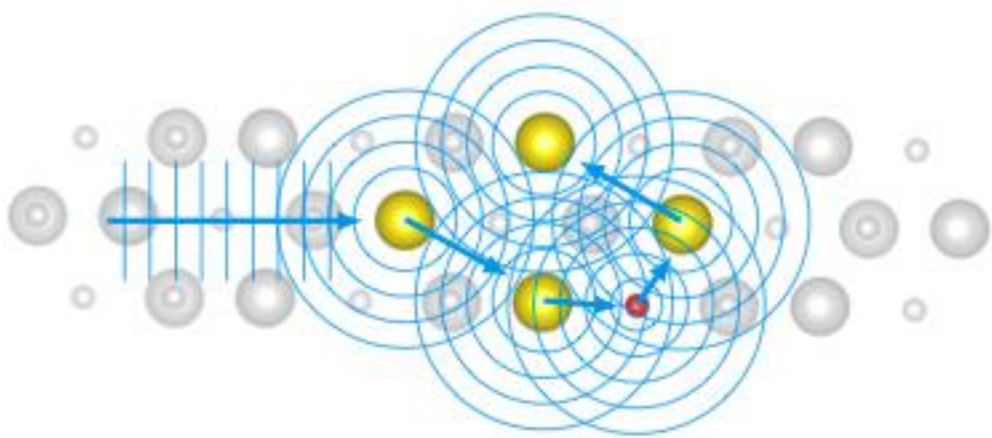
PhD (1997):
Development of a new LCAO method



Daresbury Laboratory (1997-1999)

Walter Temmerman

Balazs Gyorffy



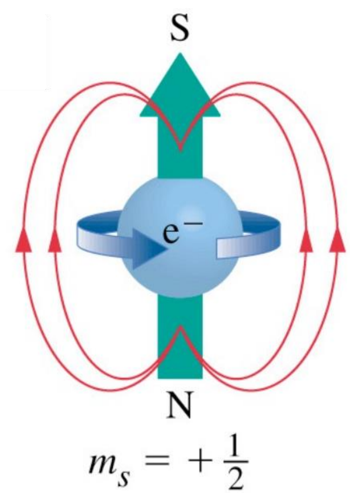
Multiple scattering theory

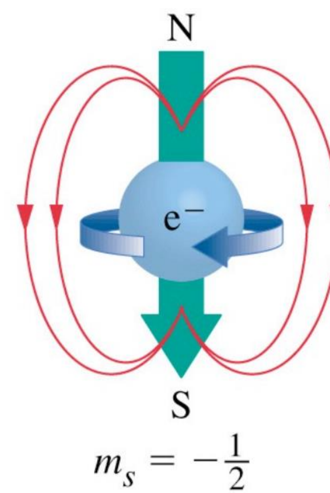
Max-Planck Institute for microstructure physics (1999-2017)

Patrick Bruno

Jürgen Kirschner

Magnetism



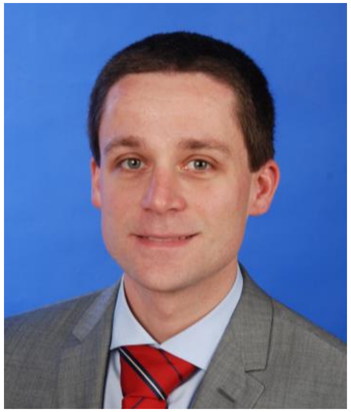


Johannes Kepler Universität Linz (since 2017)

Department for many particle physics

Helga
Böhm

Robert
Zillich



Gerhard
Tulzer

Clemens
Staudinger

Mathias
Gartner

“You can not understand it,
until you know how to calculate it.”
J. C. Slater 1900-1976

Quantum mechanical description

Erwin Schrödinger

Time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t}\Psi(\{\mathbf{r}\};t) = \hat{H}\Psi(\{\mathbf{r}\};t)$$

Describes any system

Stationary Schrödinger equation for solids:

$$\hat{H}\Psi = -\sum_{\alpha} \frac{\hbar^2}{2M_\alpha}\nabla_\alpha^2\Psi + \frac{1}{2}\sum_{\alpha\neq\beta}\frac{e^2 Z_\alpha Z_\beta}{|\mathbf{R}_\alpha - \mathbf{R}_\beta|}\Psi$$

$$-\sum_{i}\frac{\hbar^2}{2m_i}\nabla_i^2\Psi + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}\Psi - \sum_{\alpha,i}\frac{e^2 Z_\alpha}{|\mathbf{R}_\alpha - \mathbf{r}_i|}\Psi = E\Psi$$

Approximations in theoretical physics

Real cow

Approximations in theoretical physics

Real cow

Model: a spherical cow in vacuum

Approximations in theoretical physics

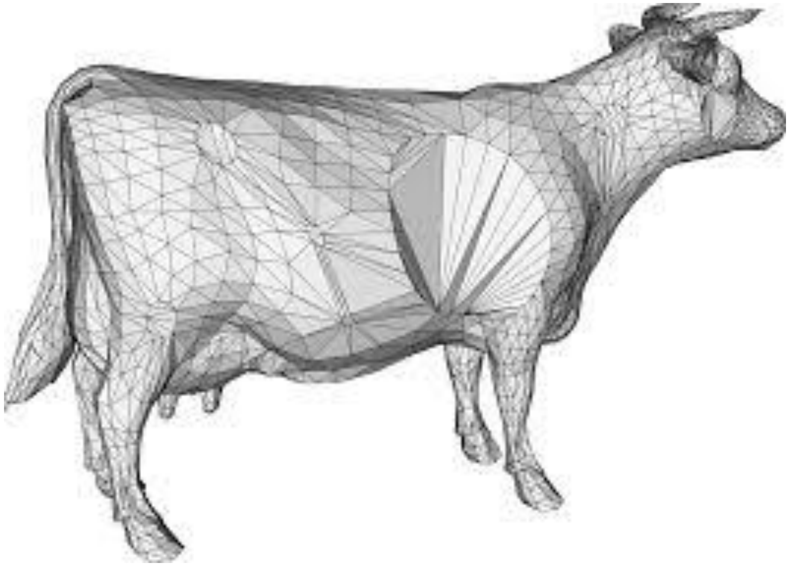
Real cow

Model: a spherical cow in vacuum

Model of interacting cows

Approximations in theoretical physics

Real cow



Realistic model:
material specific calculations

Quantum mechanical description

Problems with wave functions

- Many variables

$$\Psi(\{\mathbf{r}\};t) = \Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, ..., \mathbf{r}_N; t)$$

- Complex function
- Not measurable
- Not unique, defined up to a phase factor

Density instead wave functions (Macke 1955)

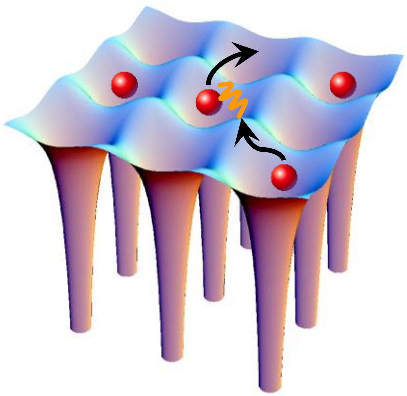
$$\rho(\{\mathbf{r}\}) = |\Psi(\{\mathbf{r}\})|^2, \;\; \rho(\{\mathbf{r}\}) \approx \rho(\mathbf{r})$$

- Measurable quantity
- Real function
- Defines unique the ground and excited states of any system

Wilhelm Macke

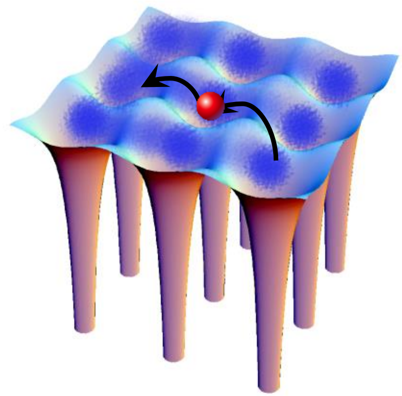
Ab-initio Computer Simulations

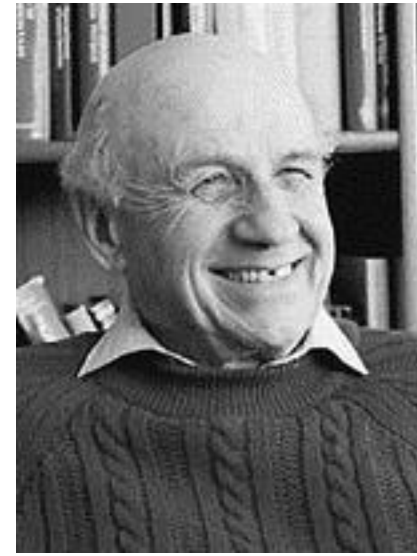
Many body problem



DFT mapping

One electron problem





W. Kohn

NP 1998

Systems

- Molecules
- Solids
- Surfaces
- Clusters

Supercomputers

Ground state properties

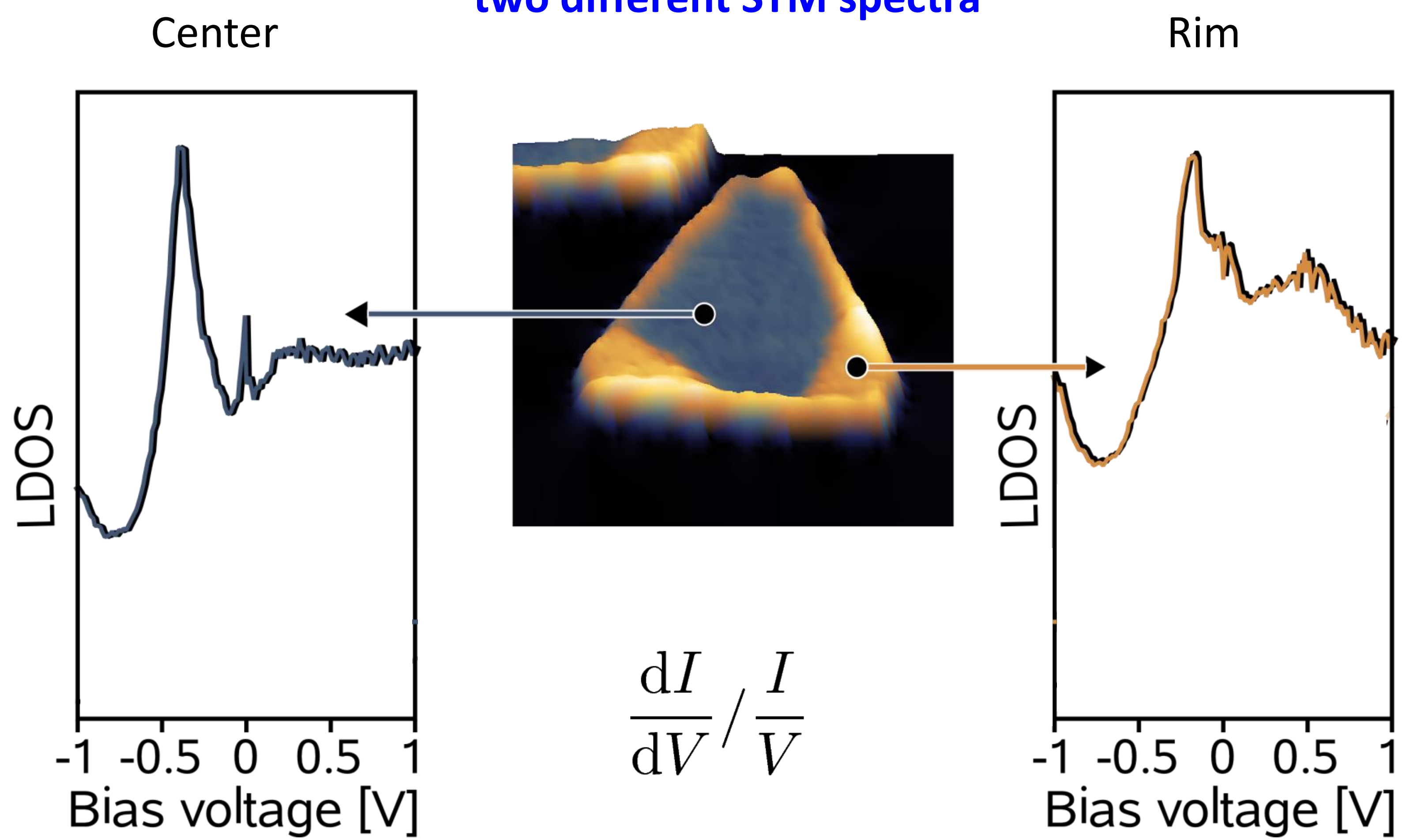
- Total energy
- Charge density

Excited state properties

- Band structure
- Magnetic excitations

Fe islands on Cu(111): STM experiment

two different STM spectra

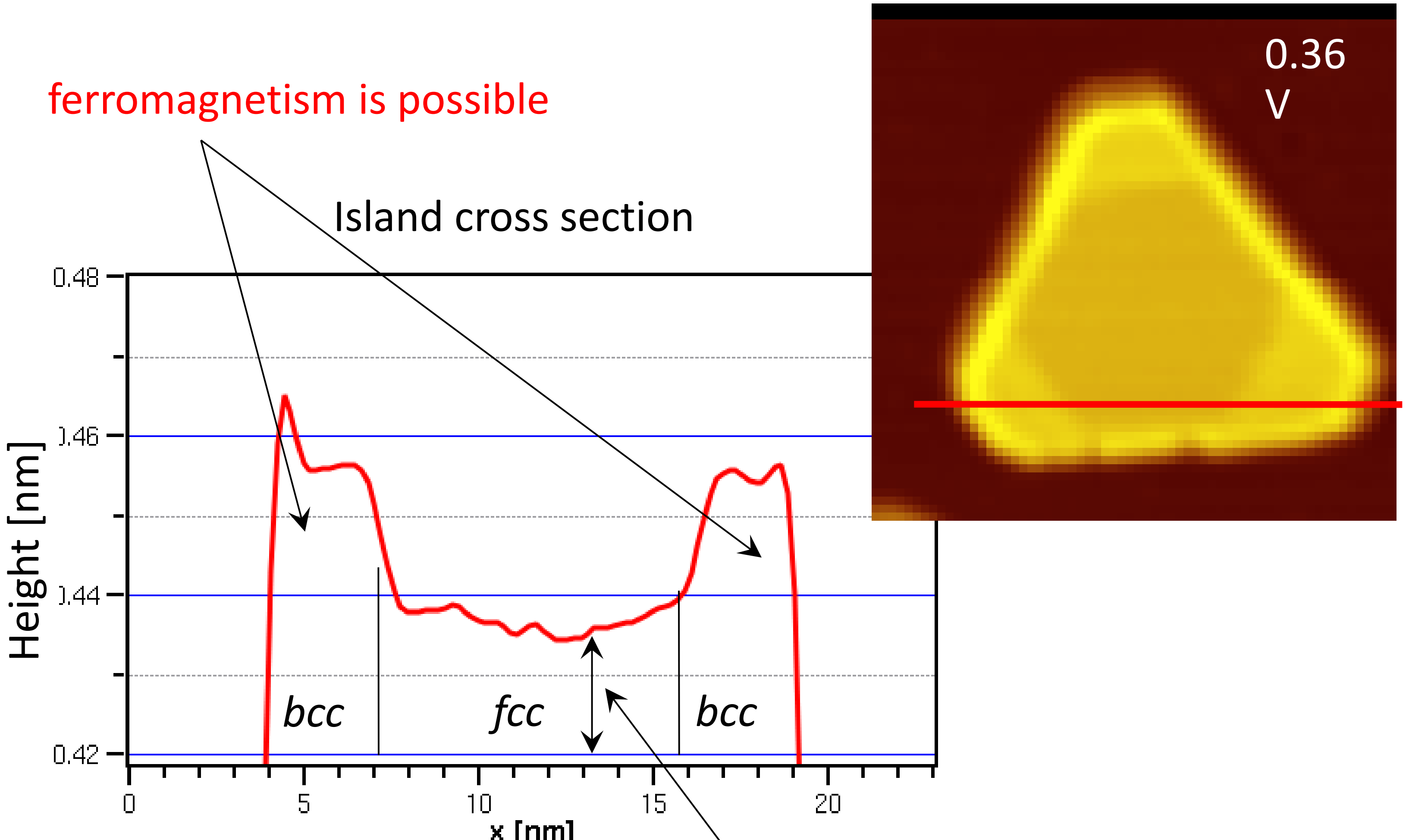


$$\frac{\mathrm{d}I}{\mathrm{d}V} / \frac{I}{V}$$

Experiment: group of Wulf Wulfhekel (TU Karlsruhe)

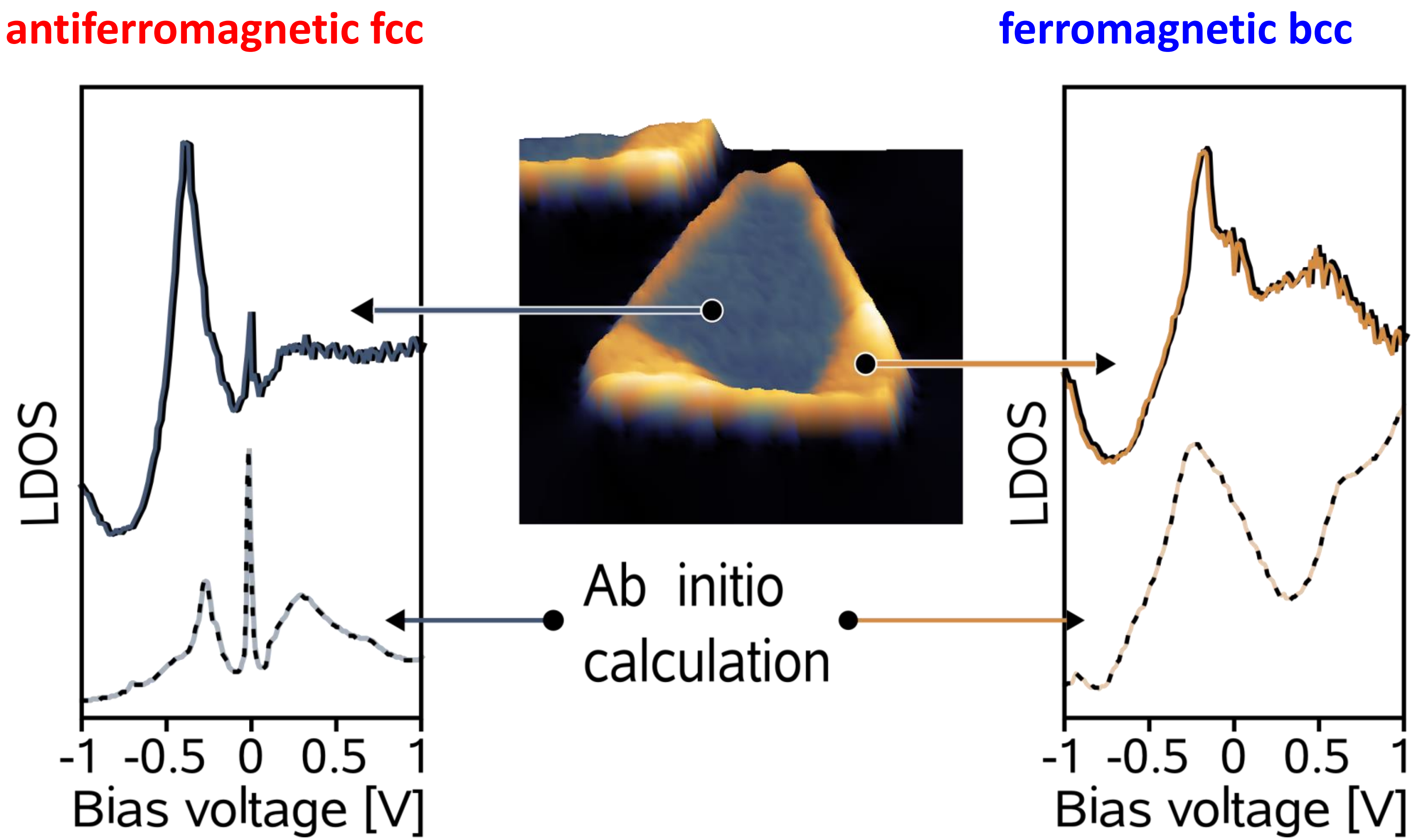
Crystallographic phases of 2ML Fe/Cu(111)

ferromagnetism is possible



reduced interlayer distance in fcc phase:
antiferromagnetism is possible

Crystallographic and magnetic phases of Fe

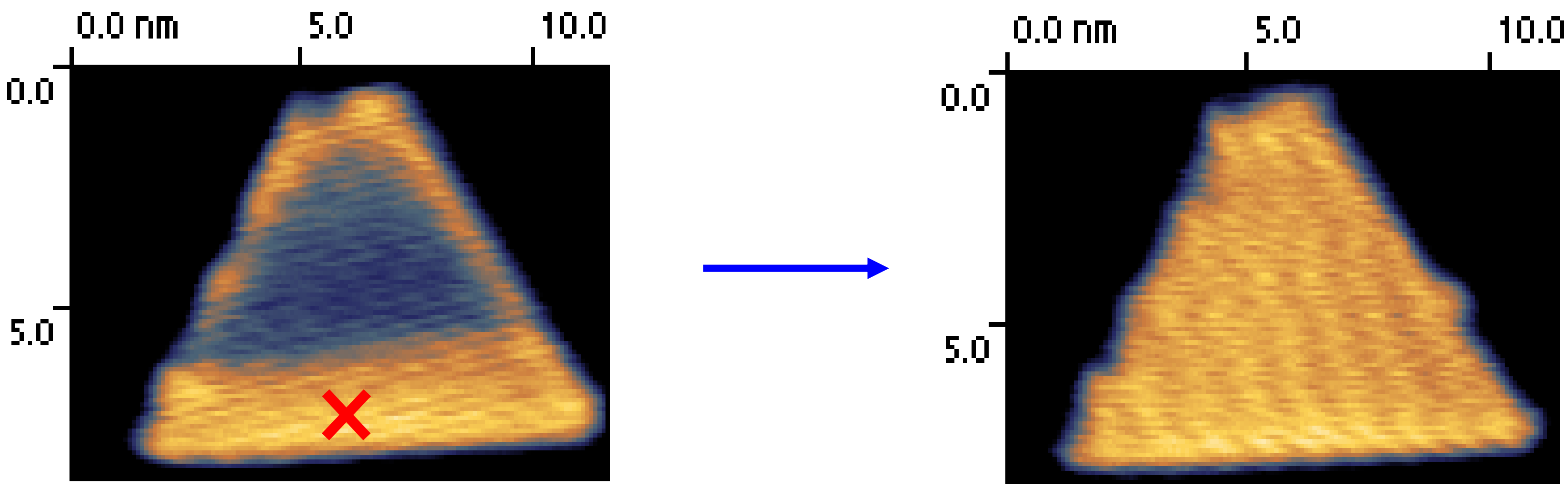


STM spectra with Tersoff-Hamann approach:

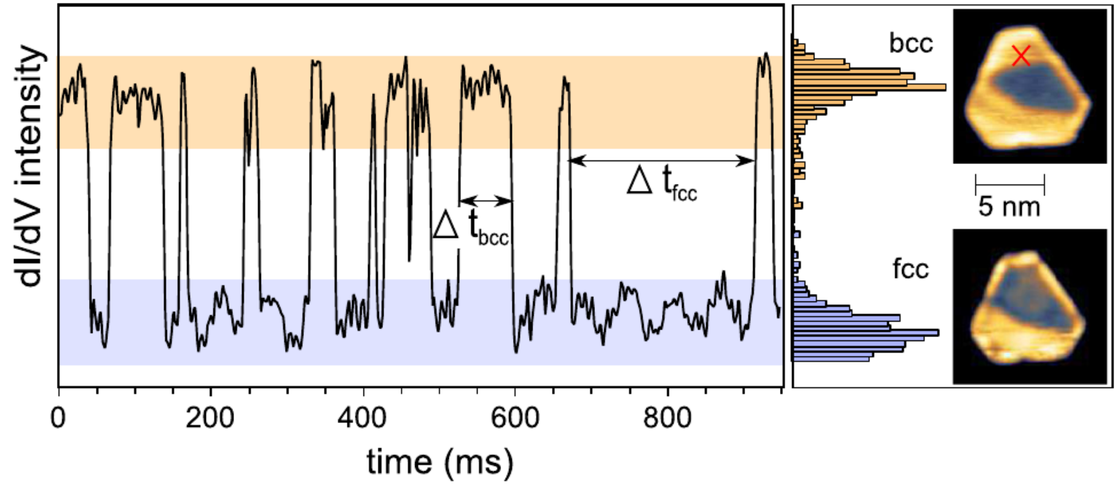
Tersoff, Hamann (1983)

Switching Fe state with an applied electric field

switching mechanism: an external electric field



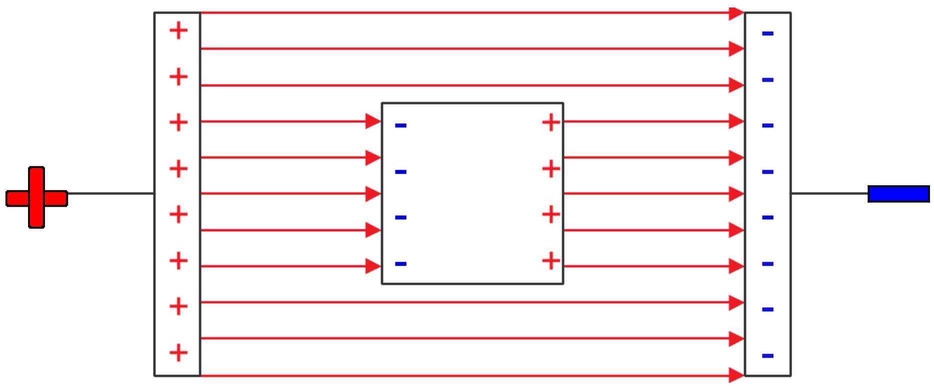
Complete islands can be switched



Metallic surfaces under an applied electric field

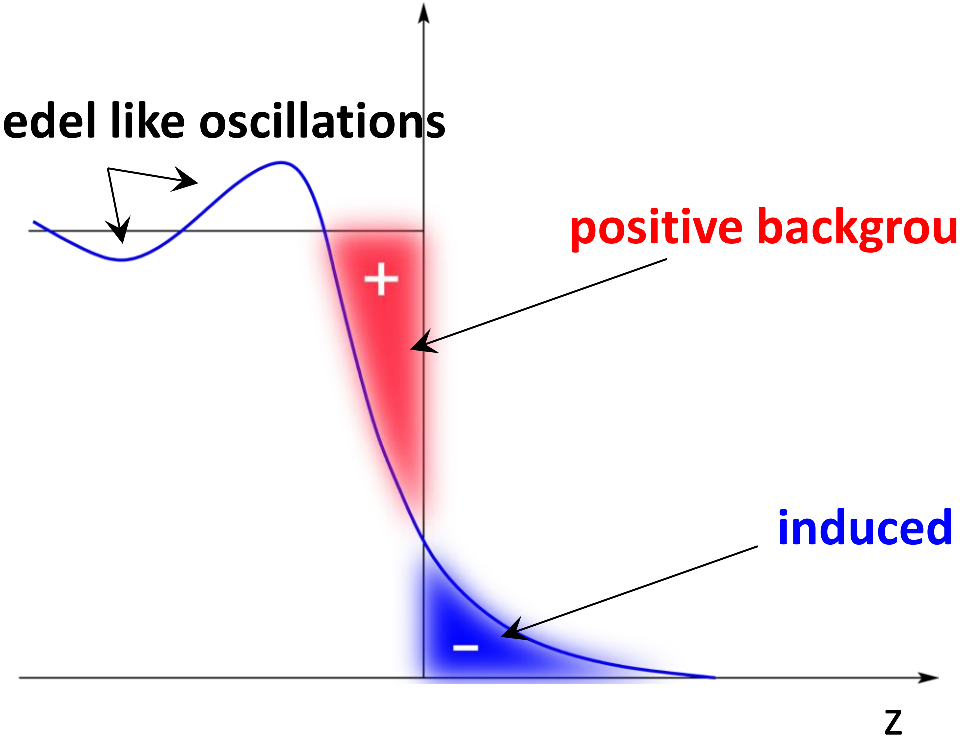
Electric field in metals

Electric field in metals is screened at the surface by free charge carriers



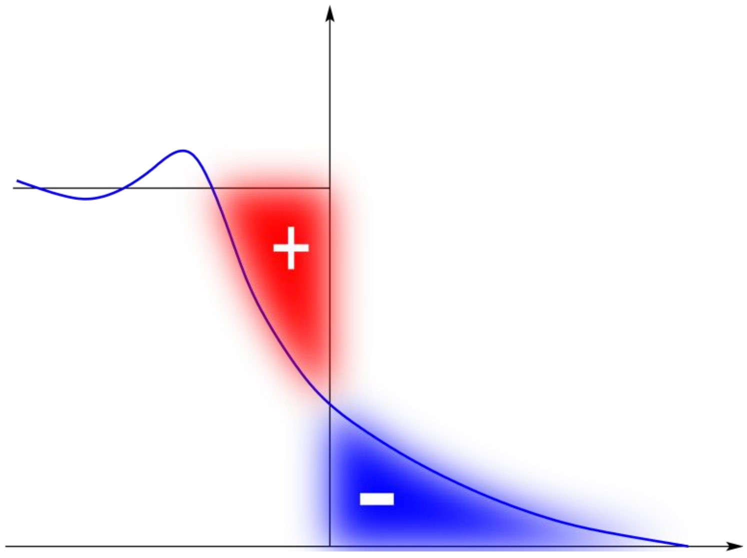
Charge density in vicinity of a surface (Lang & Kohn 1971)

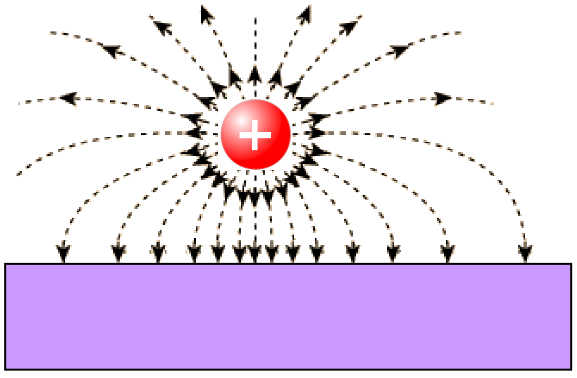
Friedel like oscillations



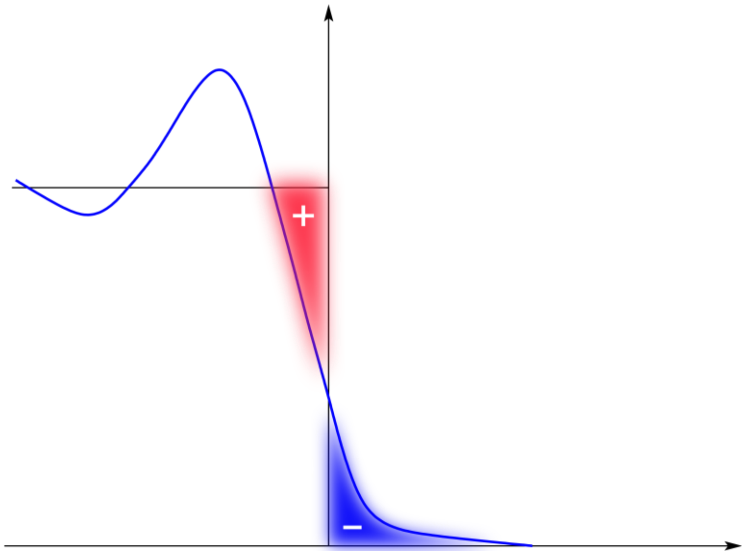
Formation of a surface dipole

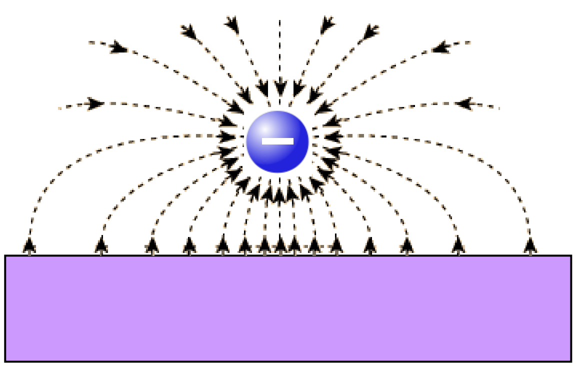
Metallic surface under an applied electric field



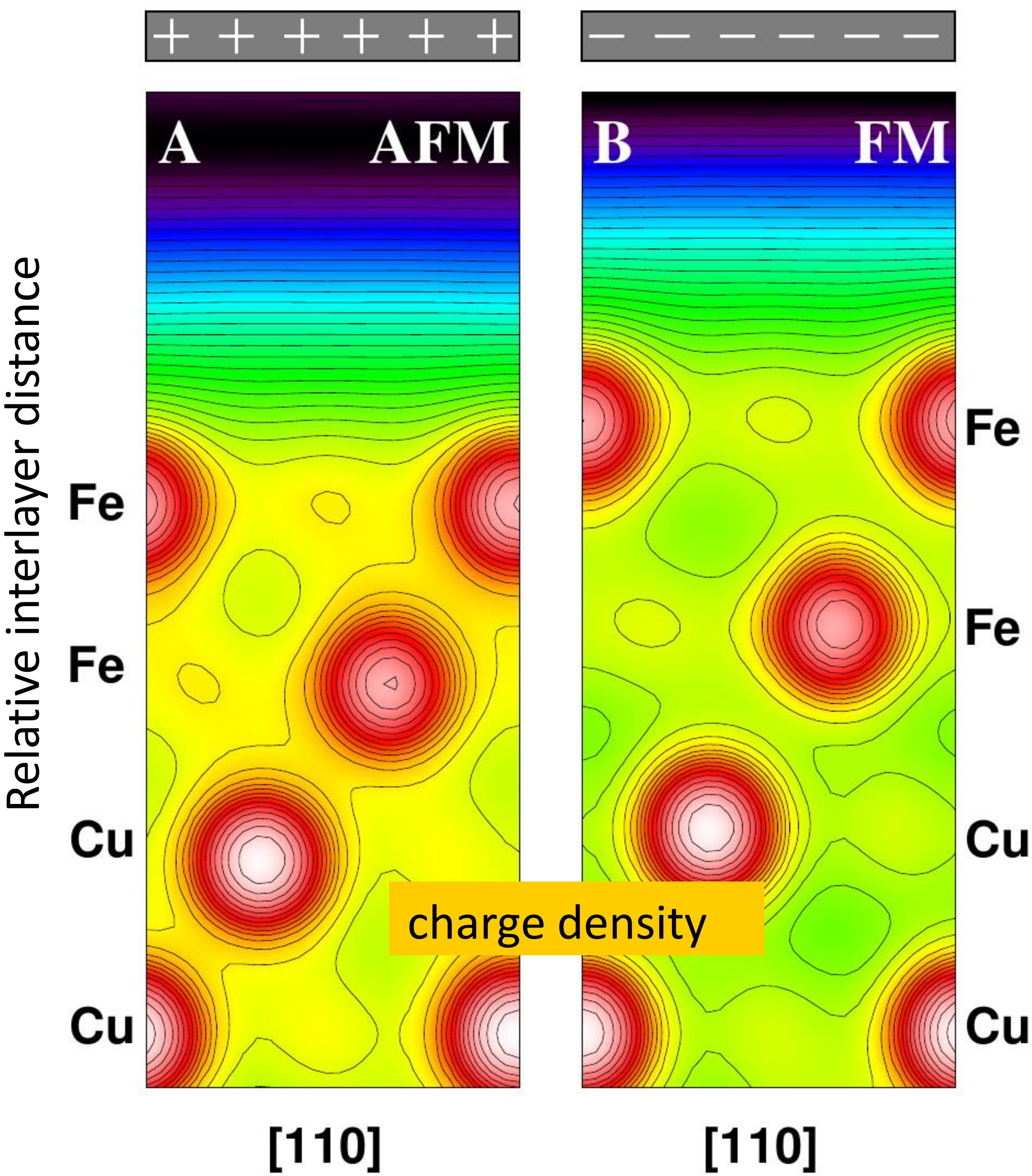


Change of the dipole barrier induces atomic relaxations in the vicinity of the surface

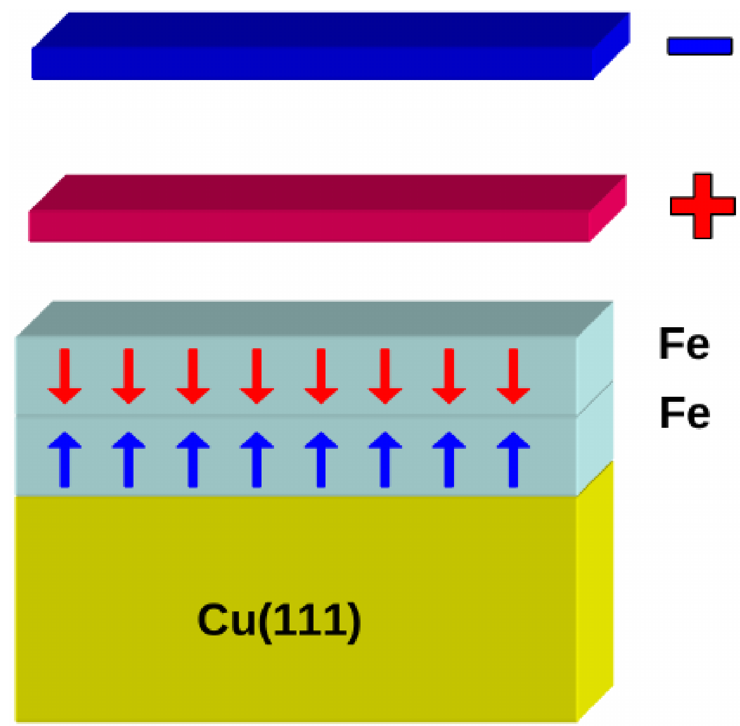




Layer relaxations under an applied electric field



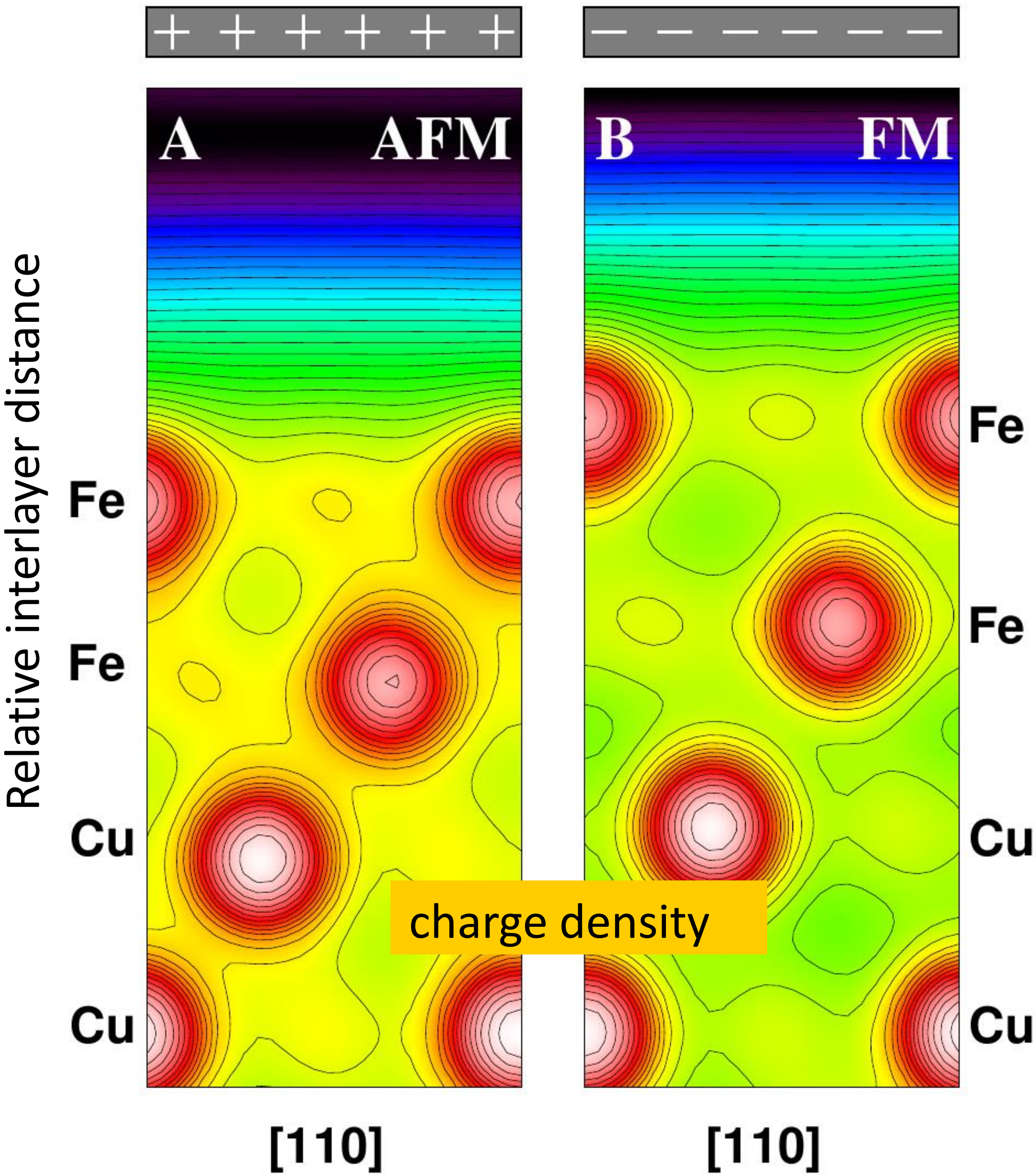
First-principles simulations



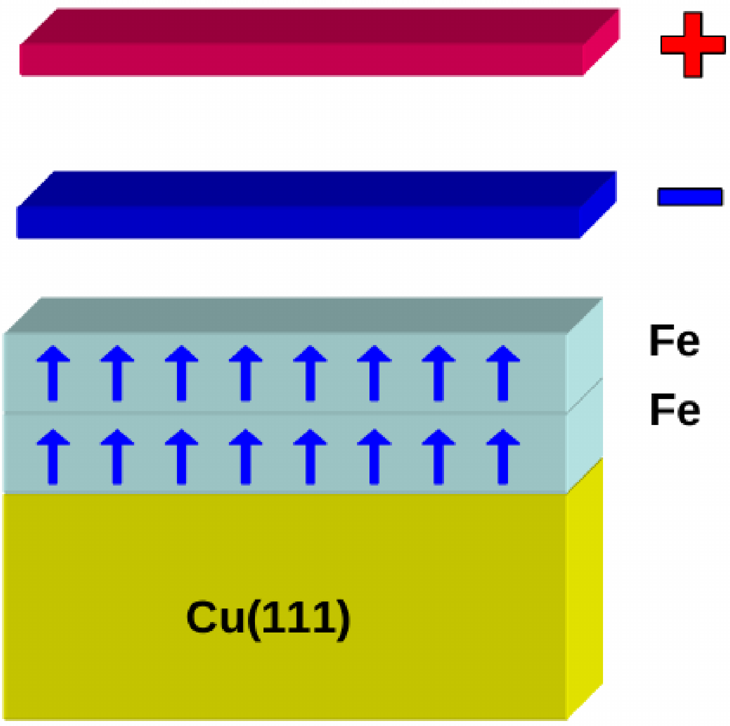
only vertical displacements

Antiferromagnetic order

Layer relaxations under an applied electric field



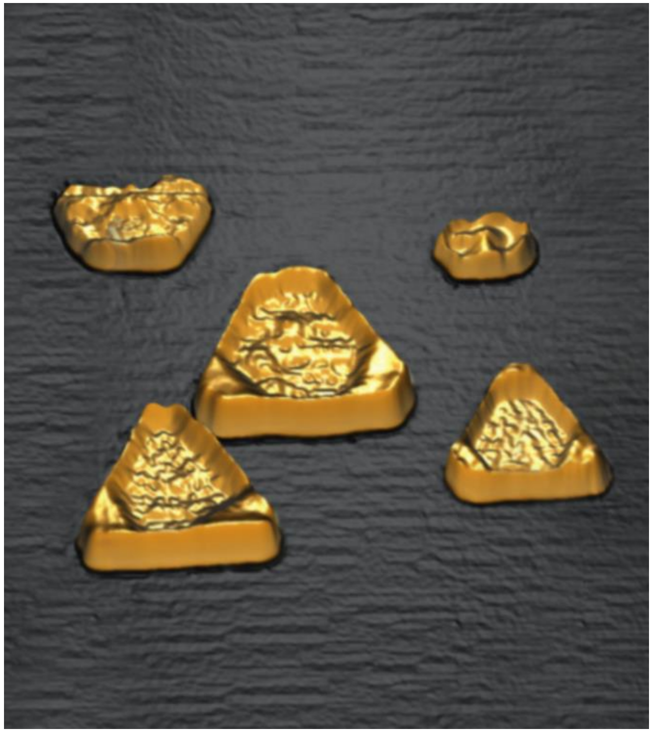
First-principles simulations



only vertical displacements

Ferromagnetic order

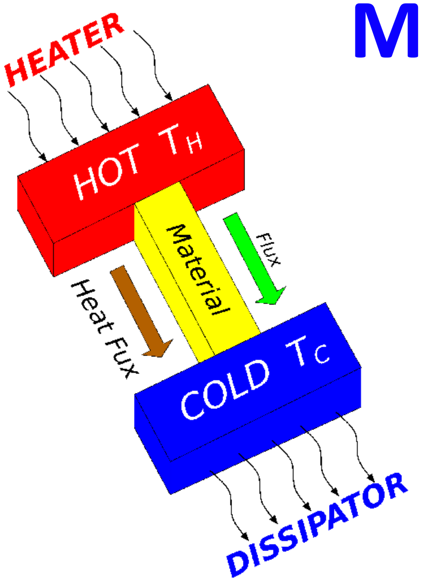
Fe islands as a memory device switchable by an electric field



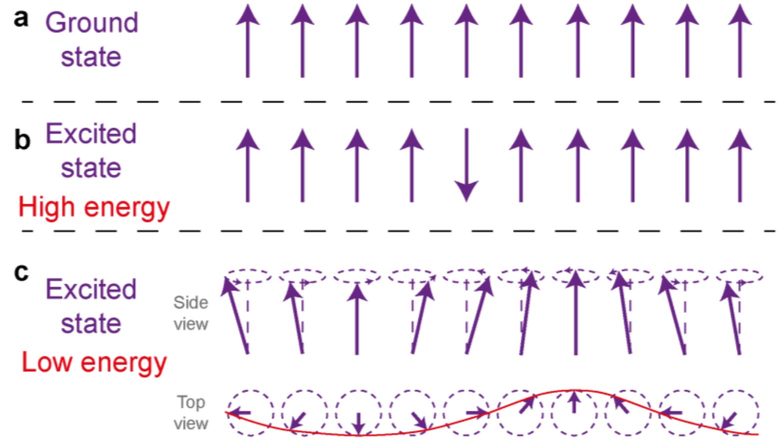
Capacity: 400-600 larger then in conventional memory devices

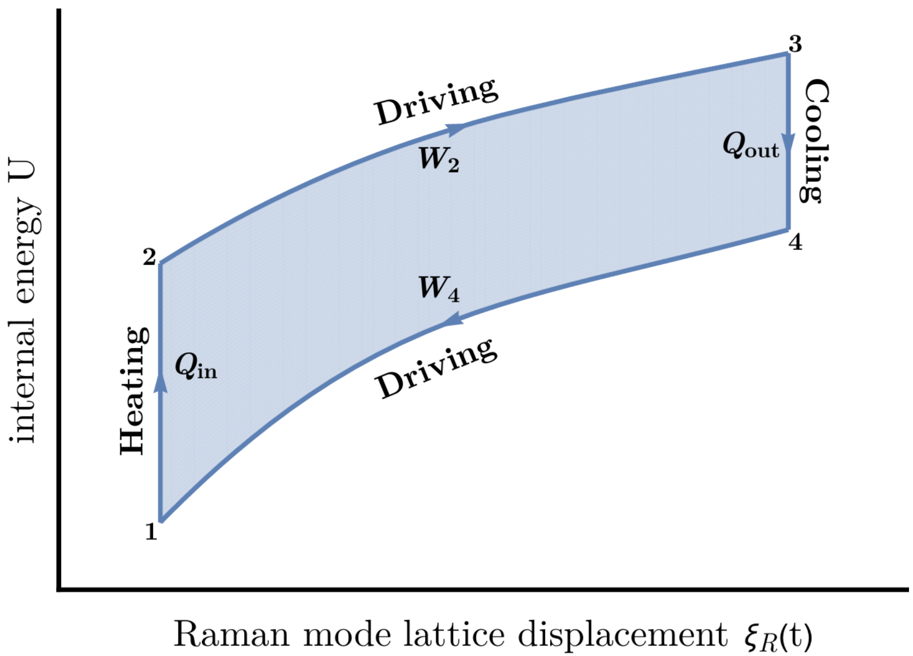
L. Gerhard, T. K. Yamada, T. Balashov, A. F. Takacs, R. J. H. Wesselink, M. Däne, M. Fechner, S. Ostanin, A. Ernst, I. Mertig and W. Wulfhekel
Nature Nanotechnology (2010)

Magnon-driven quantum heat engine

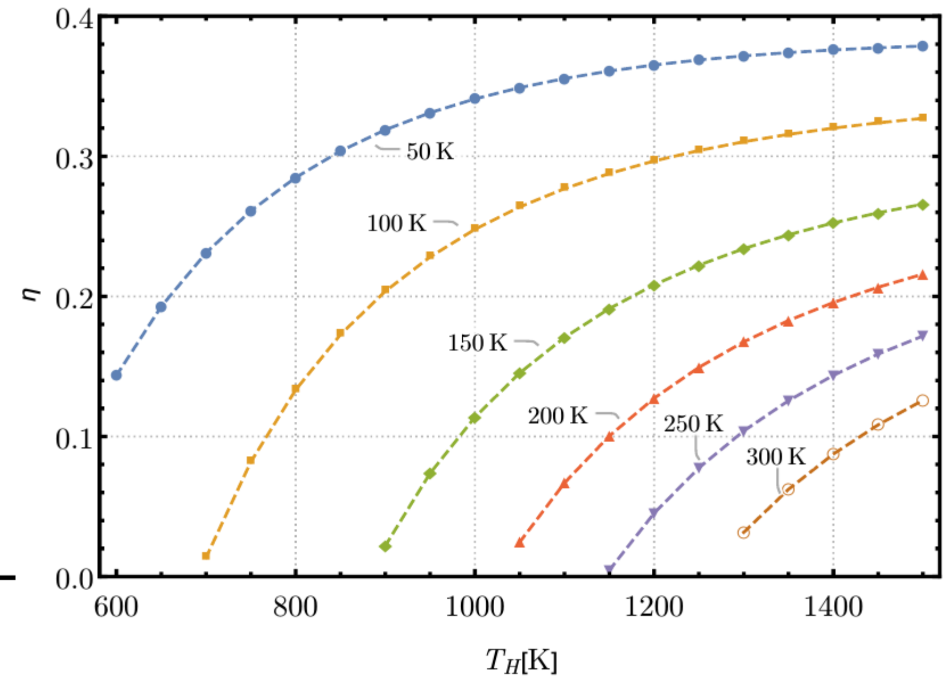


Magnons





Efficiency of the heat engine

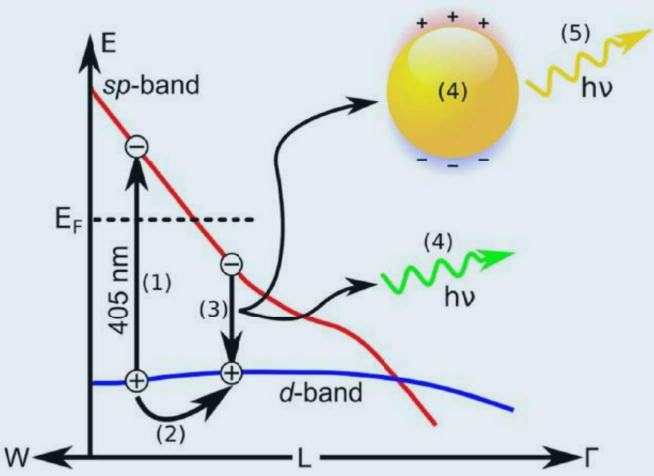


Gerhard Tulzer, Levan Chotorlishvili, Martin Hoffmann, Robert Zillich

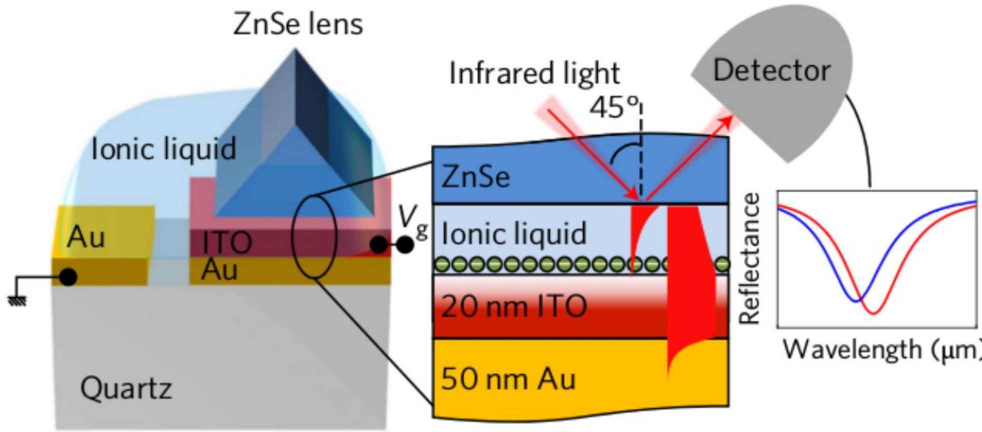
Surface plasmons

Motivation: experiments made by the group of Thomas Klar

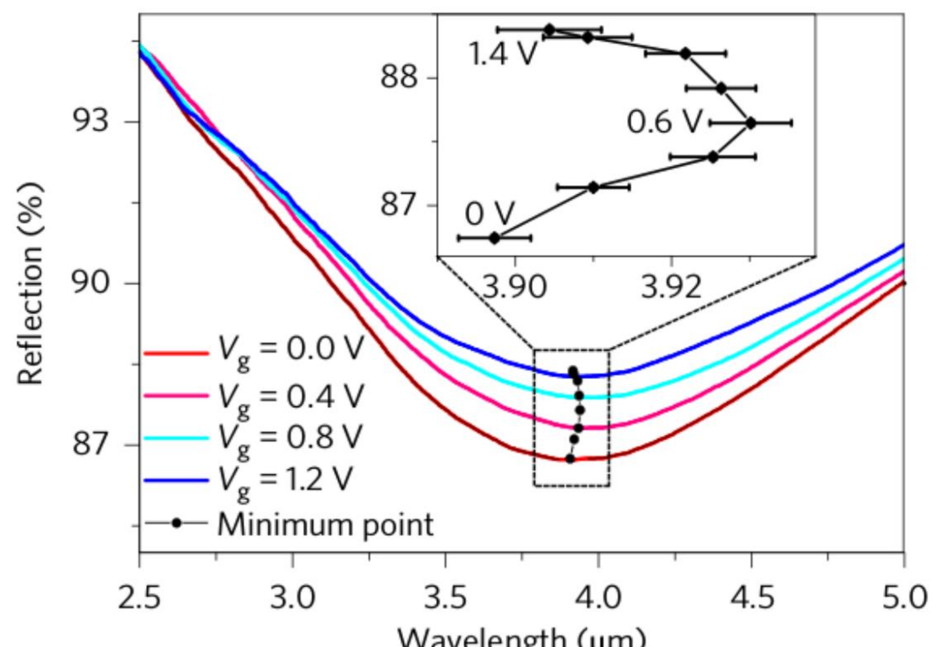
Plasmons in nanoparticles



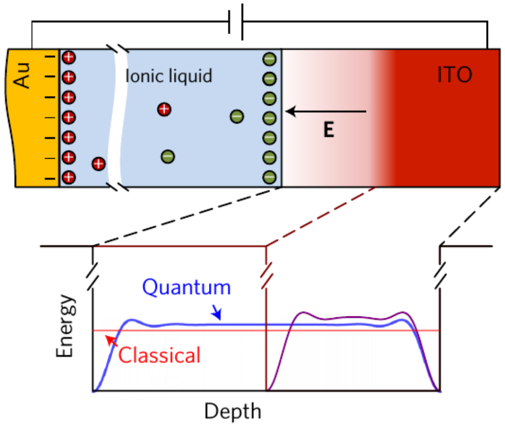
D. Sivun (Thesis, 2017)

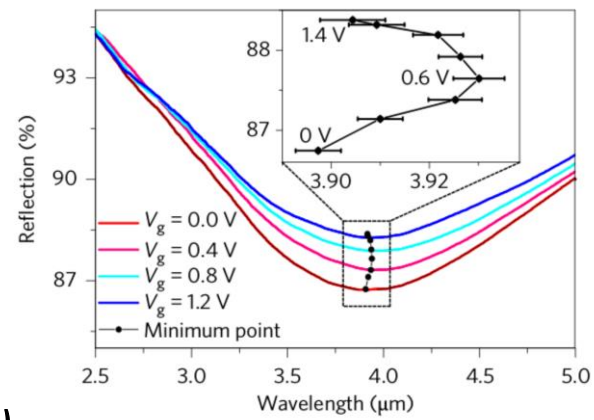


X. Liu et al. (2017)



Surface plasmons



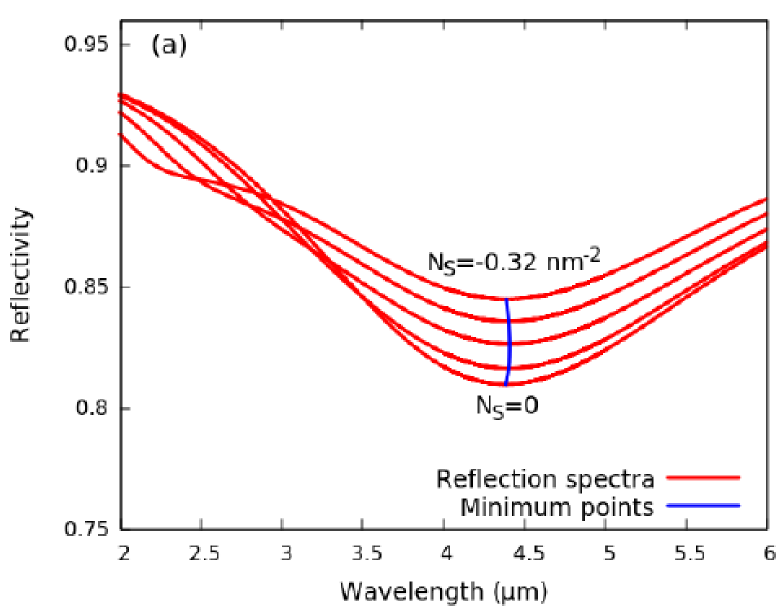


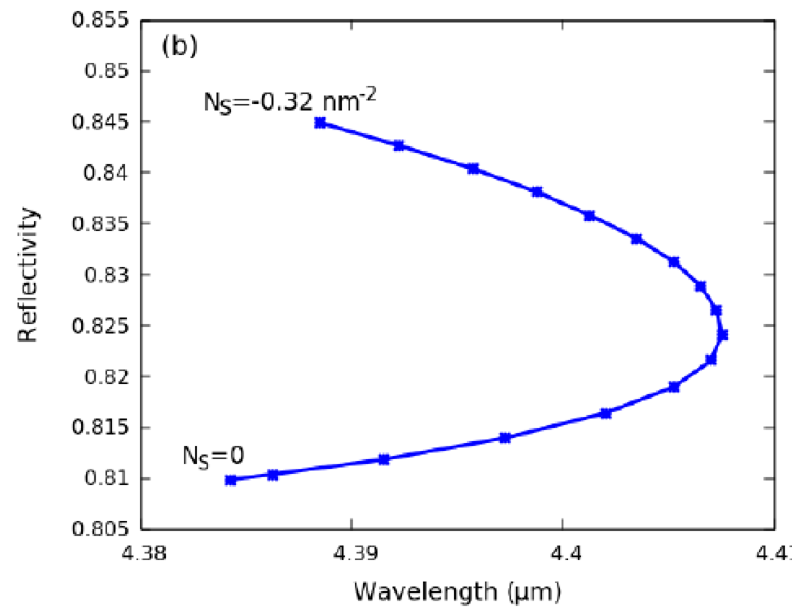
Experiment: X. Liu et al. (2017)

David Kurunczi-Papp

Theory:

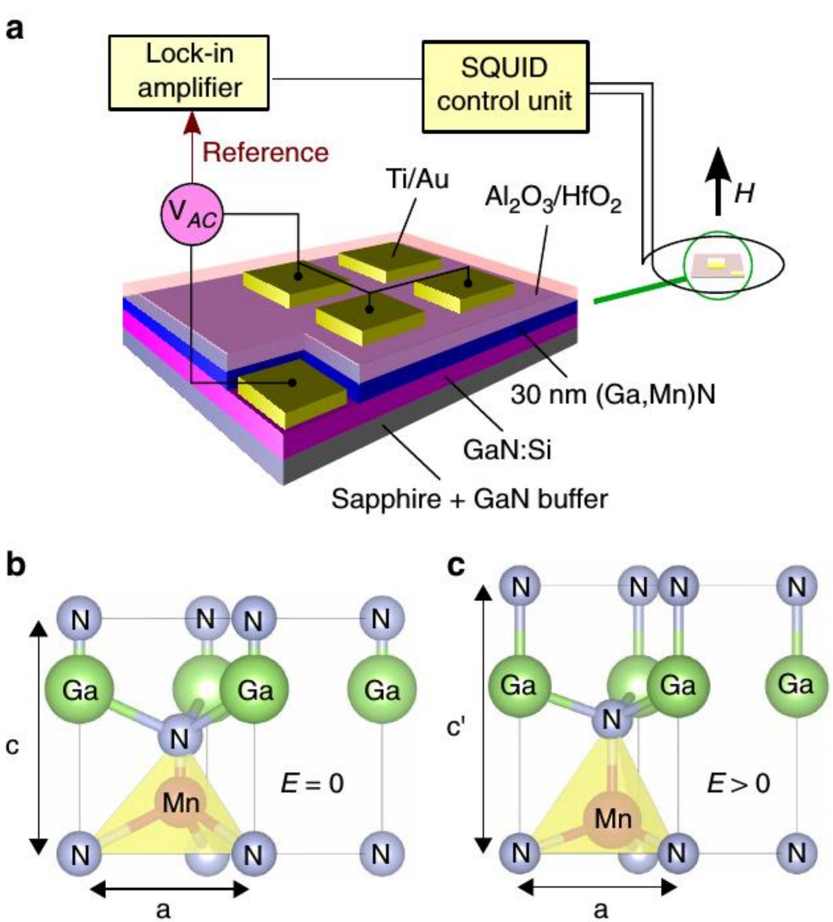
- Quantum mechanical description
- Proper boundary conditions



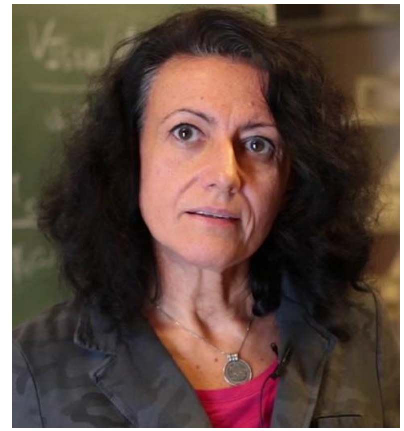


Tuning magnetism with an electric field

Motivation: experiments made by the groups of A. Bonanni and A. Ney



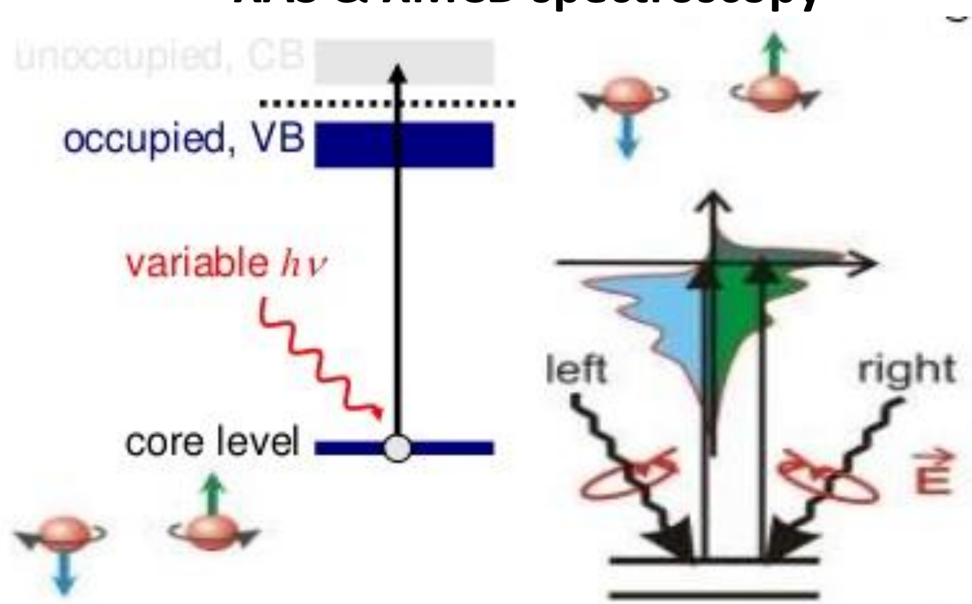
D. Sztenkiel et al. (2016)



Alberta Bonanni

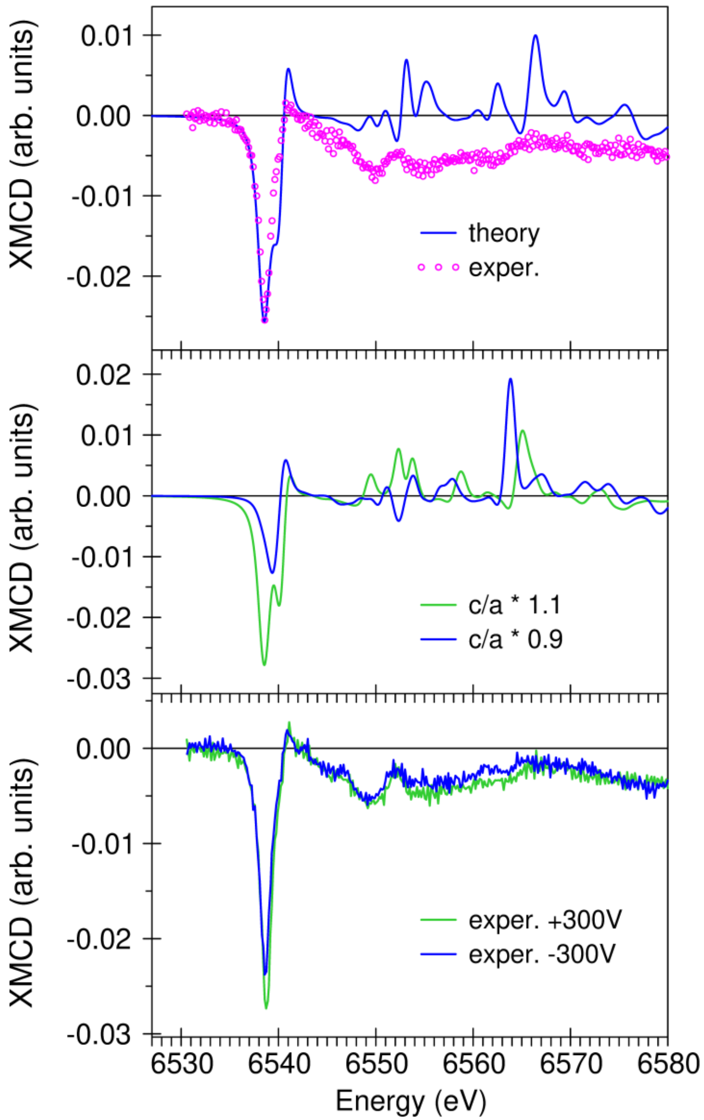
Andreas Ney

XAS & XMCD spectroscopy

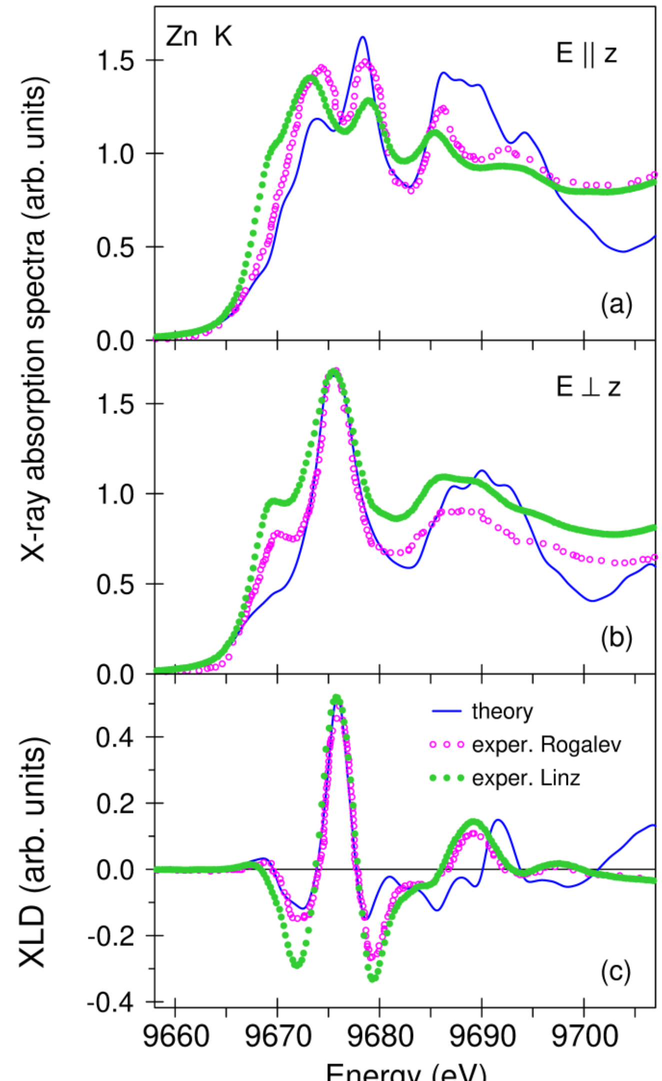


Tuning magnetism with an electric field: GaMnN & ZnCoO

Mn K edge in GaMnN

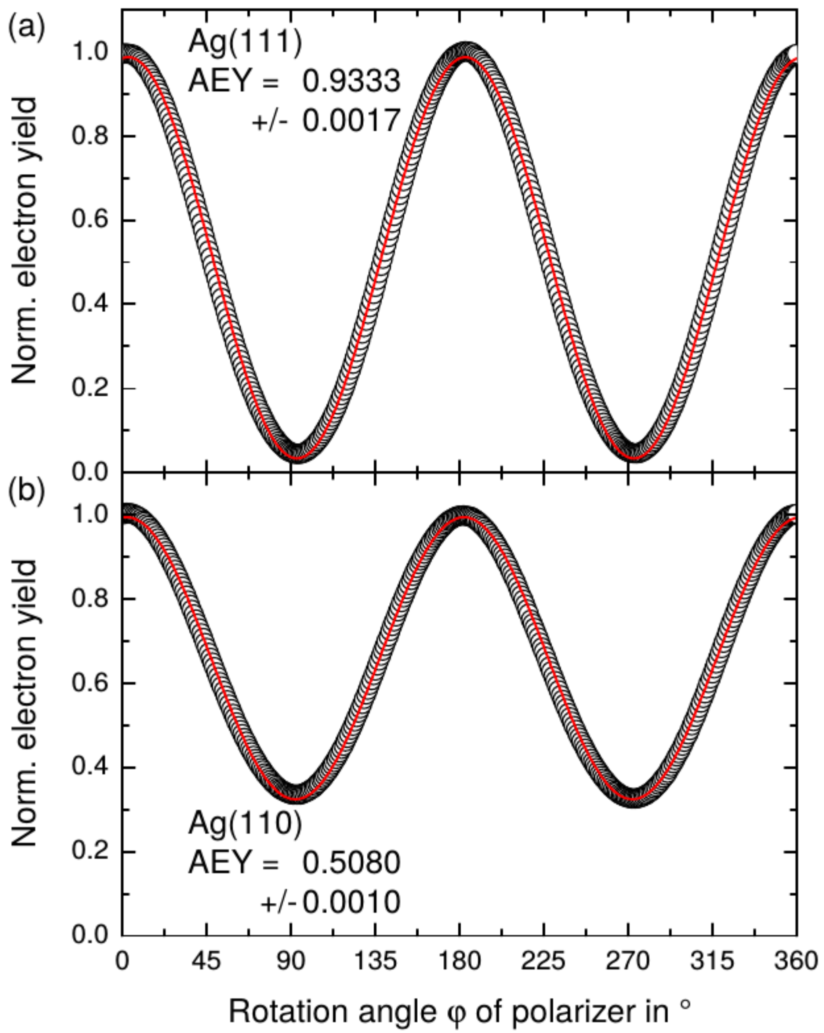


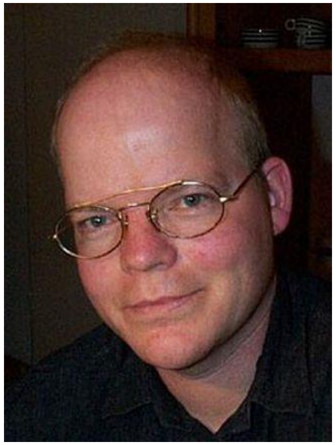
Zn K edge in ZnCoO



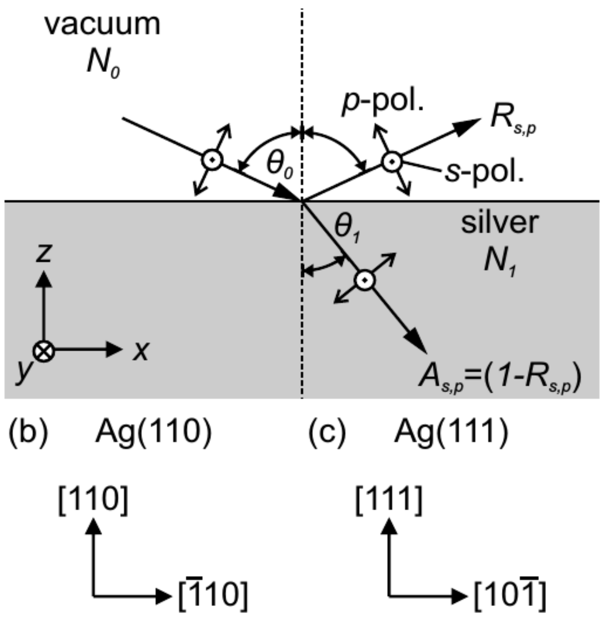
Photoemission from Ag(110) and Ag(111) surfaces

Polarization dependency of PE for various Ag surfaces



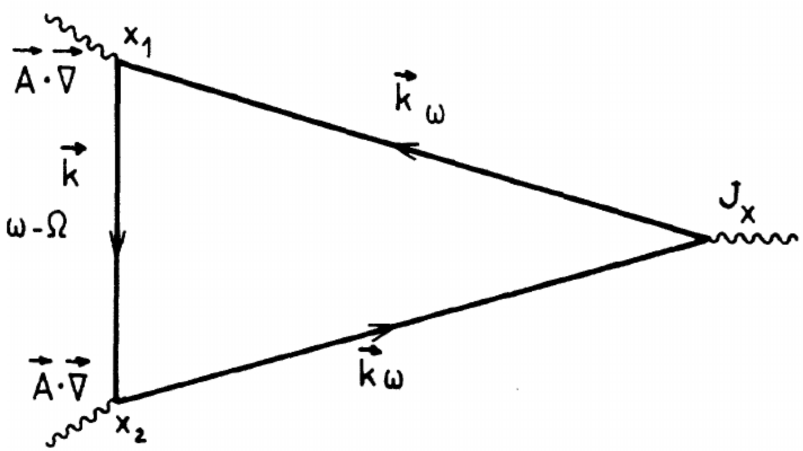



Thorsten Wagner Peter Zeppenfeld



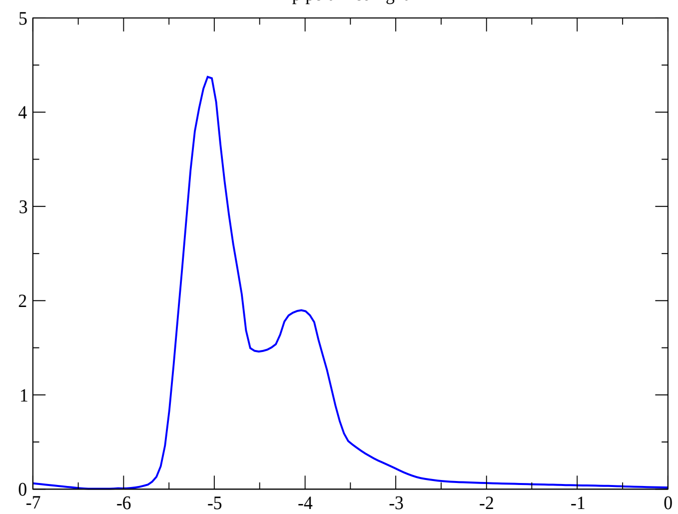
Photoemission from Ag(110) and Ag(111) surfaces

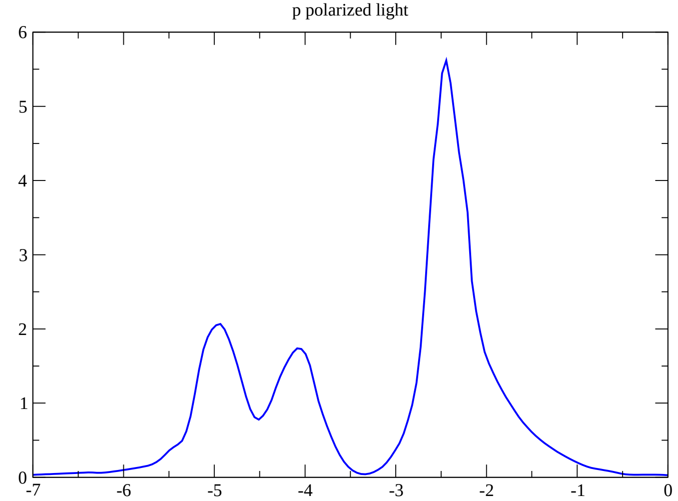
Theory: Fermi Golden rule



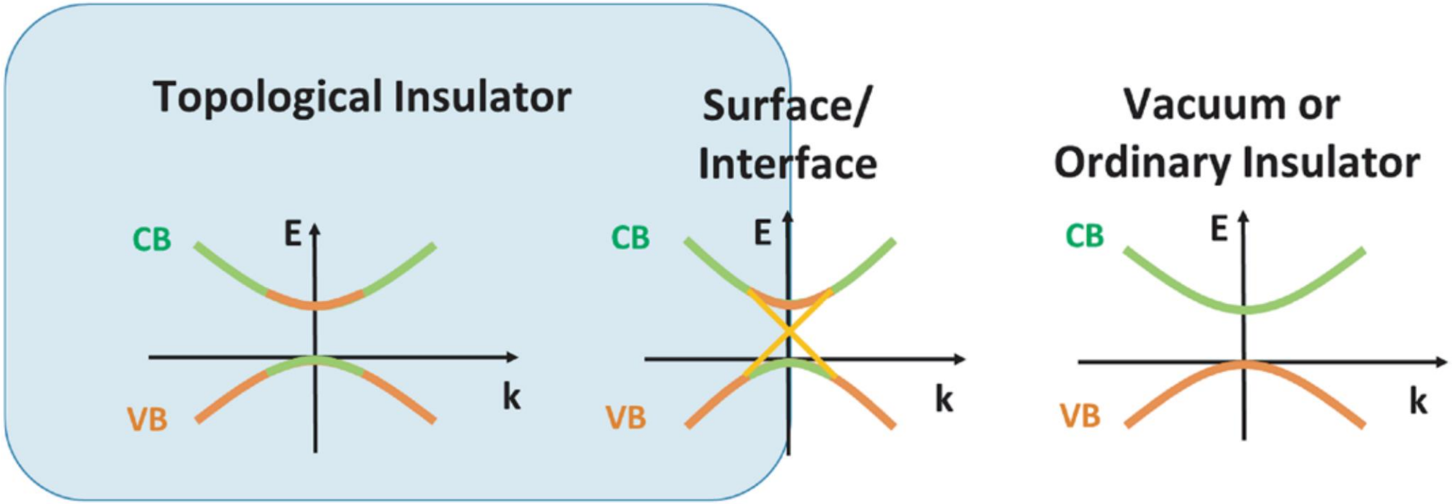
$$w_{fi} = \left|\langle \Phi(\boldsymbol{k}_{\|}, E_f) \middle| \Delta \middle| \Psi_i \rangle\right|^2 \delta(E_f - E_i + \omega)$$

Simulations of PE from first-principles



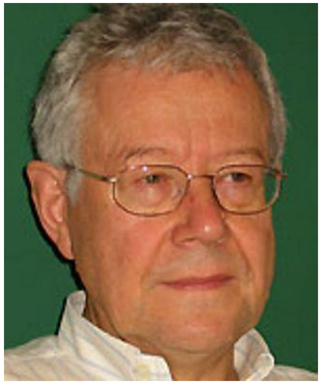


Topological insulators

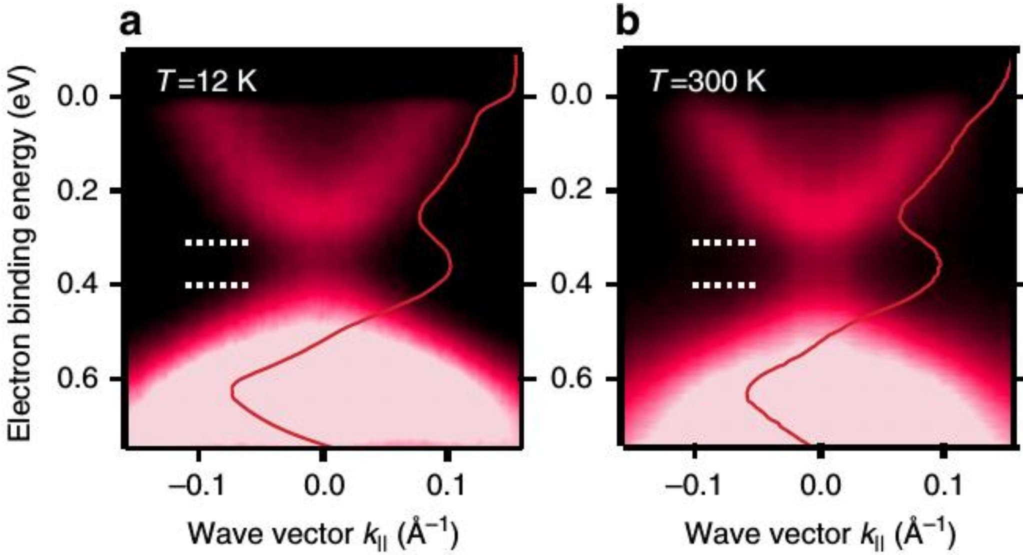


Motivation: experiments made by the groups of G. Springholz and G. Bauer

Gunther Springholz

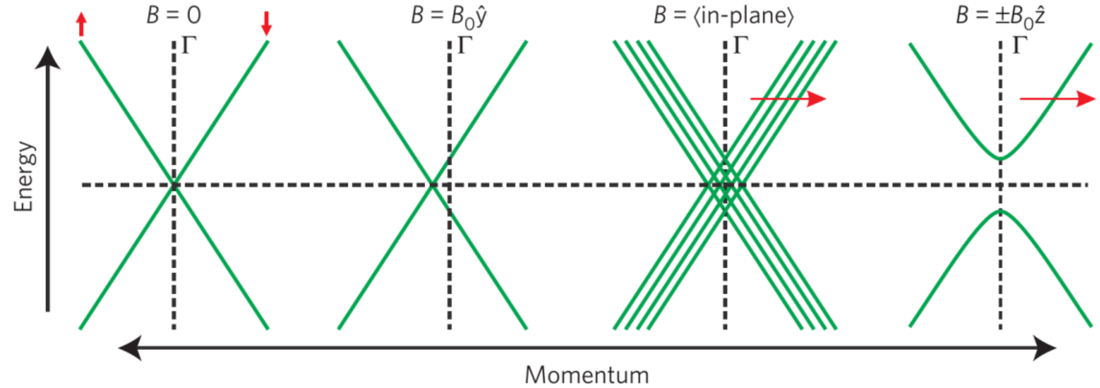


Günther Bauer

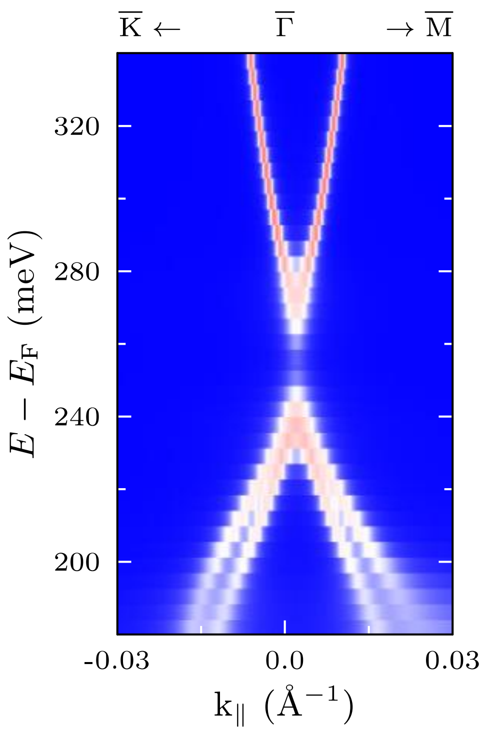


Mn in Bi_2Se_3: *J. Sanchez-Barriga et al. (2015)*

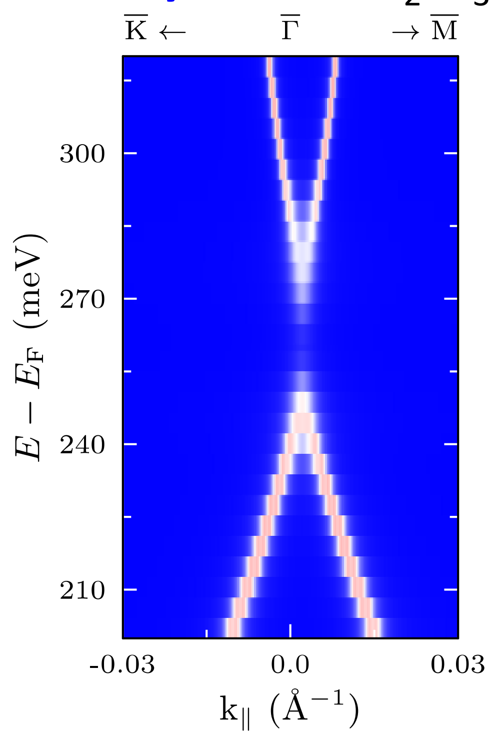
Topological insulators



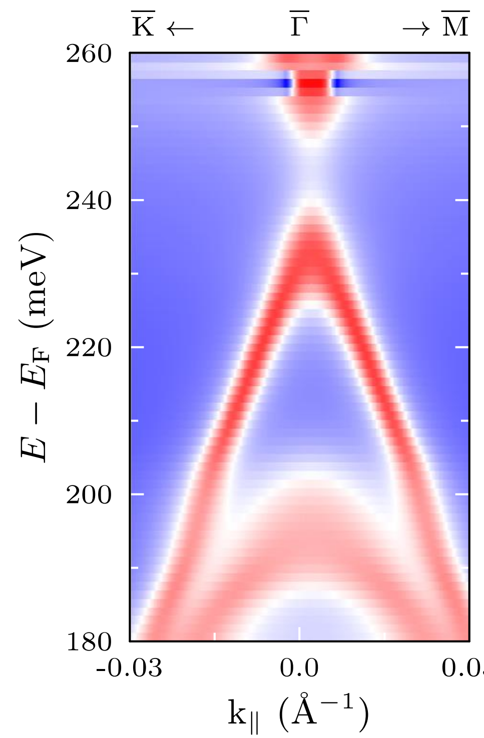
Theory: Mn in Bi_2Se_3



Magnetic case



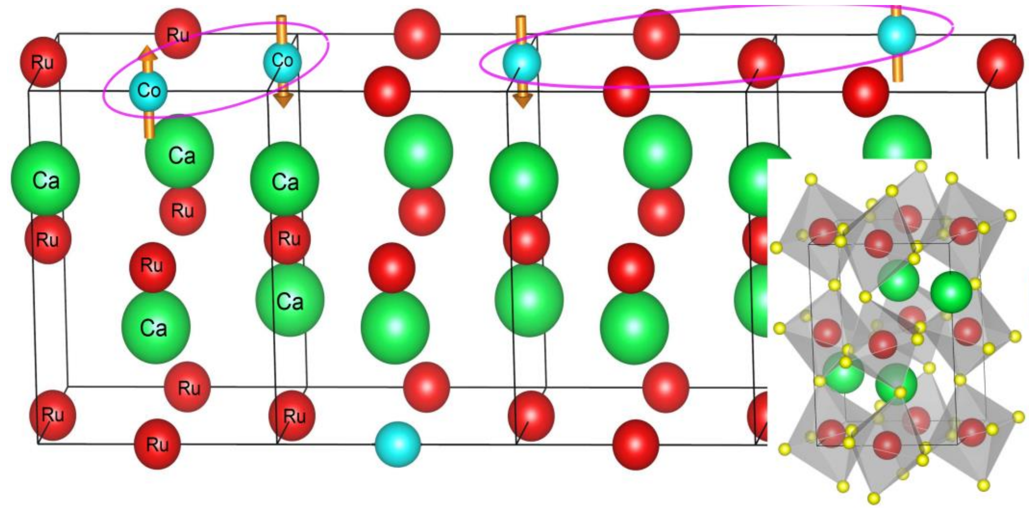
Paramagnetic case



Nonmagnetic case

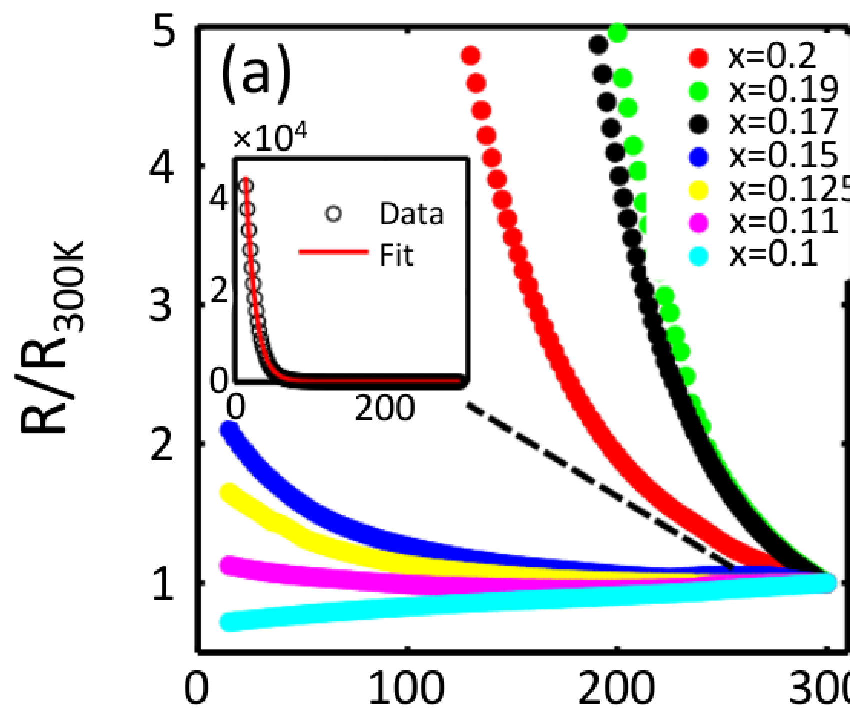
Metal-Insulator transition in $CaRu_{1-x}Co_xO_3$

Deepak Singh

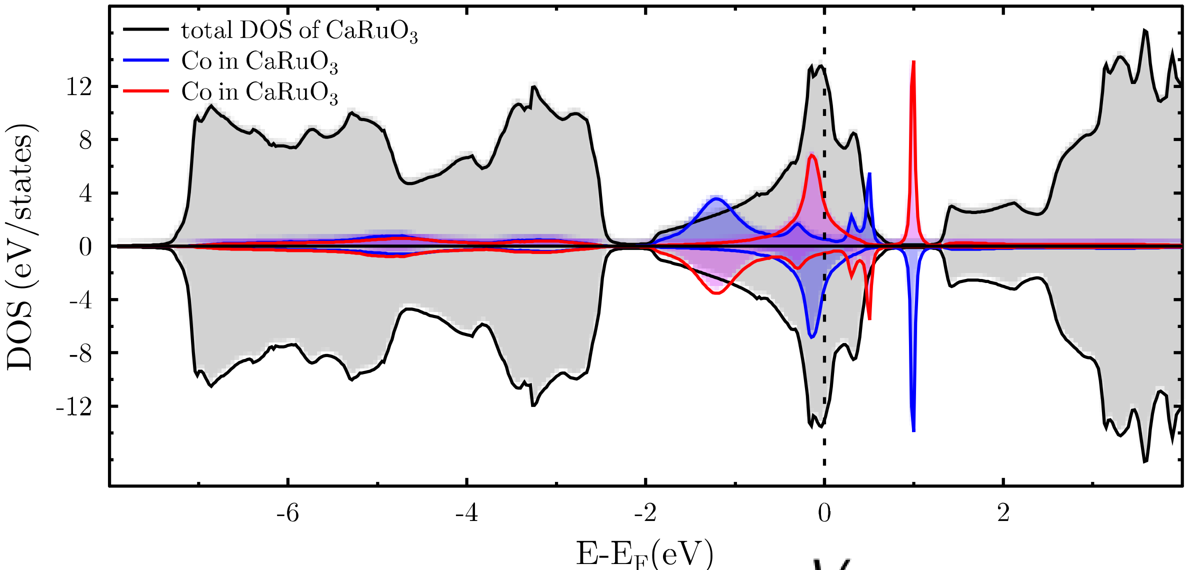


Experiment

- for x < 0.15 - metallic
- at x = 0.15 - coexistence of a weak spin glass phase with the quantum spin liquid-type state
- for 0.15 < x < 0.27 - insulator
- for x > 0.27 - phase separation in the structure

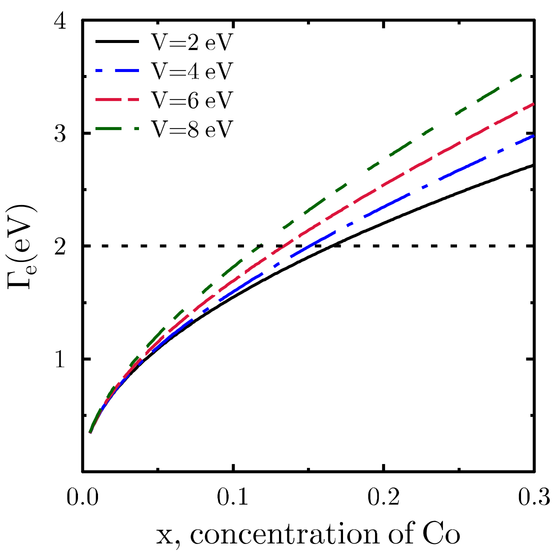


Anderson model for $CaRu_{1-x}Co_xO_3$



Florian Sipek

$$H = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \frac{V}{\sqrt{N_0}} \sum_{\mathbf{k}i} \left(a_{\mathbf{k}}^{\dagger} a_i + h.c. \right) + \sum_i \varepsilon_i a_i^{\dagger} a_i$$

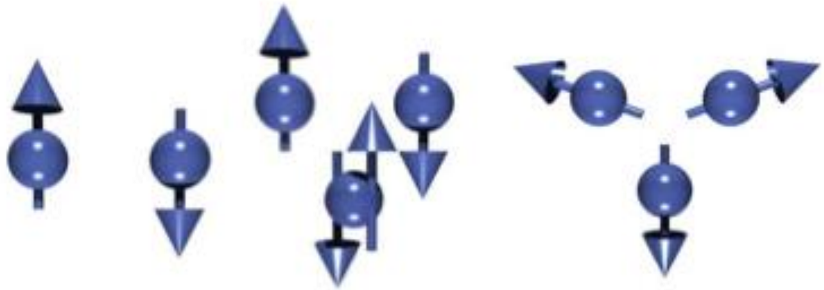


$$\Sigma_e = \frac{xV^2}{\varepsilon - \varepsilon_i + i\Gamma_i}$$

$$\frac{\hbar}{2\tau_e} \equiv \Gamma_e = \frac{xV^2\,\Gamma_i}{(\varepsilon - \varepsilon_i)^2 + \Gamma_i^2}$$

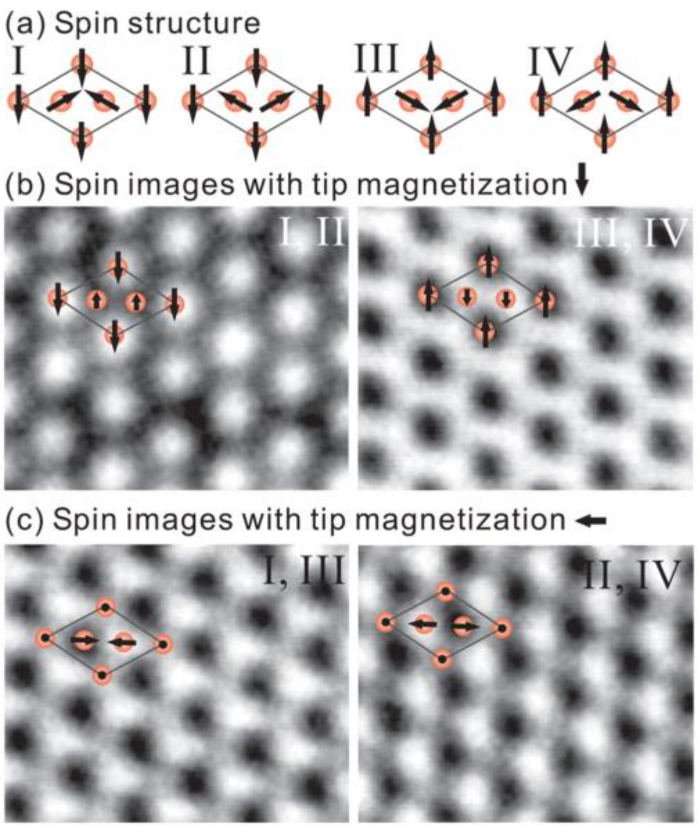
Martin Hoffmann

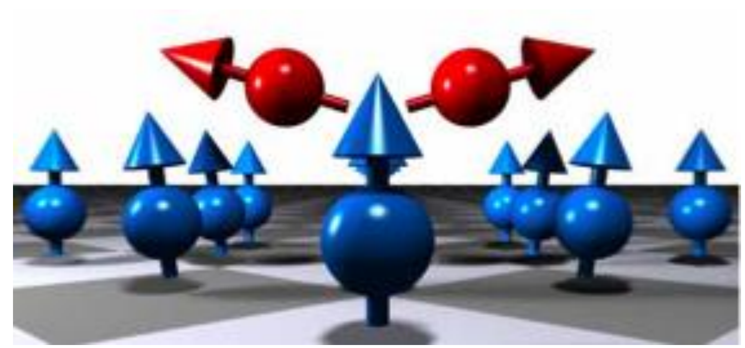
Non-collinear magnetism



Collinear and non-collinear magnetic structures

David Eilmsteiner



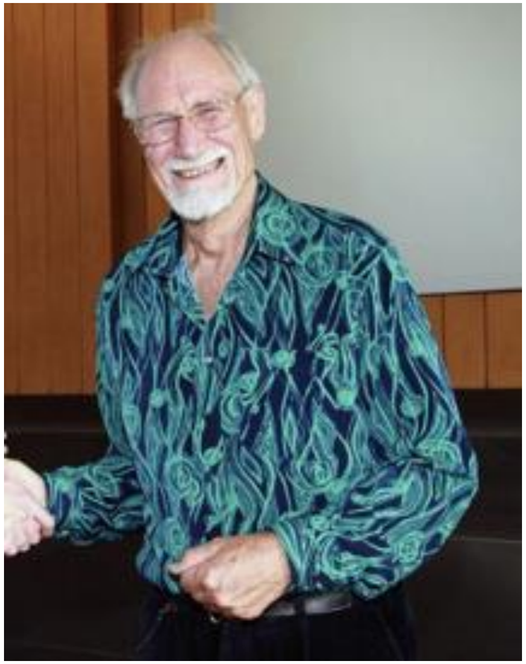


Experiment: Mn on Ag (111) surface

S. Gao, W. Wulfhekel (2010)

“How often I have read a paper about a piece of computational physics which finishes with the words... and we obtain good agreement with experiment. If you know the answer from experiment, I want to cry, why are you wasting so much of time calculating it?“

Volker Heine



Thank you very much for your attention