

DFT-based Green function approach for impurity calculations

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Challenge: quantum description of materials

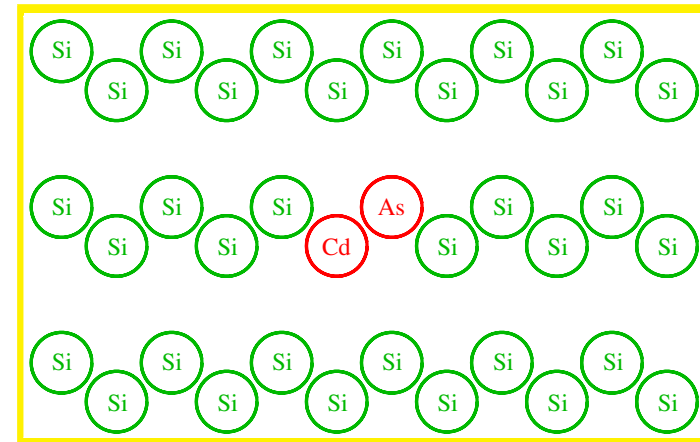
materials contain atoms which consist of electrons and nuclei

laws of quantum mechanics determine the properties

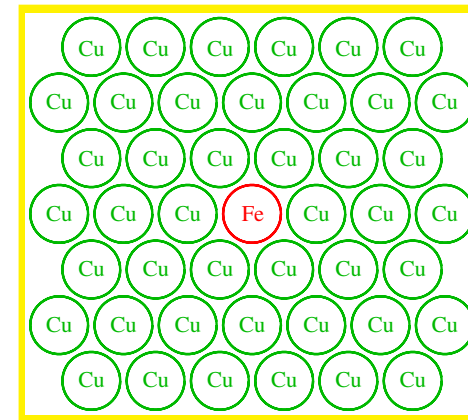
Pauli, Schrödinger, Heisenberg and Dirac (1925-1928)

approximations are necessary

CdAs complex in Si



Fe impurity in Cu



Electronic structure calculations

Born-Oppenheimer approximation (fixed nuclei) \Rightarrow

$$\mathcal{H}\Psi = E\Psi$$

$$\mathcal{H} = -\sum_i^N \nabla_i^2 + \sum_{i<j}^N \sum e^2 |\underline{r}_i - \underline{r}_j|^{-1} + \sum_i^N v_{\text{ext}}(\underline{r}_i)$$

many electron Schrödinger equation $N \approx 10^{23}$

Hohenberg-Kohn theorem: all properties are determined by **density** $n_0(\underline{r})$

$$v_{\text{ext}}(\underline{r}) \Rightarrow \Psi \Rightarrow n_0(\underline{r}) \Rightarrow v_{\text{ext}}(\underline{r})$$

ground-state energy $E_0 = \min_n E[n(\underline{r})]$

Kohn-Sham equations

auxiliary system without interaction $e^2 = 0$ with same density $n(\underline{r})$
 \Rightarrow single-particle equations with effective potential $v_{\text{eff}}(\underline{r})$

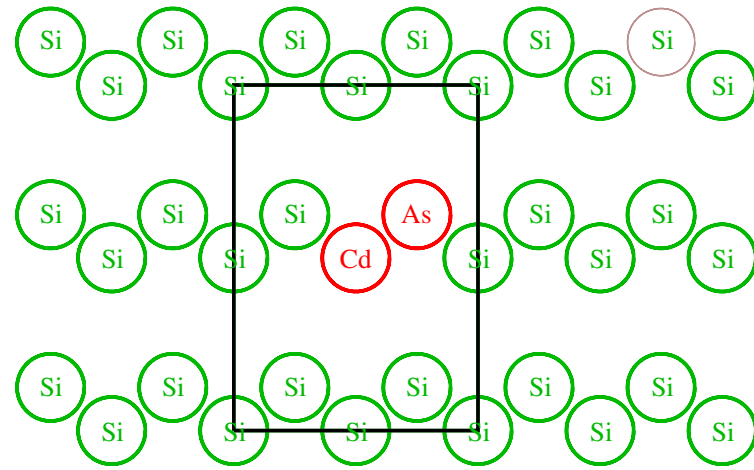
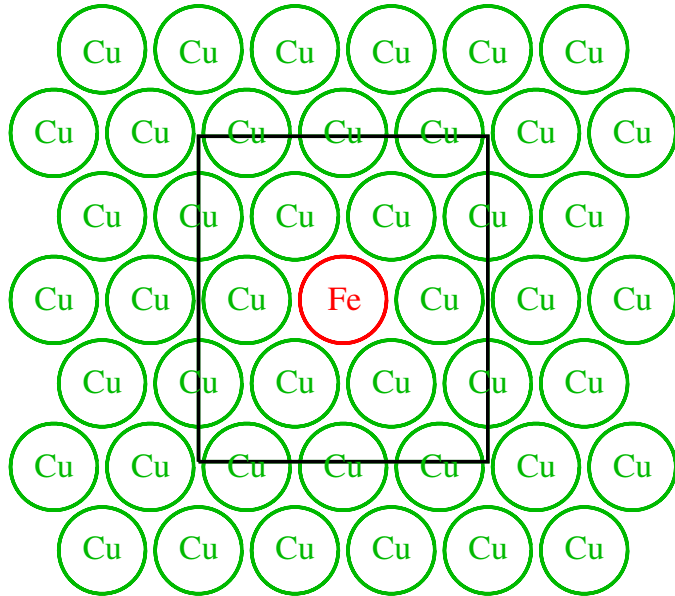
$$n(\underline{r}) = \sum_i |\varphi_i(\underline{r})|^2$$

$$[-\nabla_{\underline{r}}^2 + v_{\text{eff}}(\underline{r})]\varphi_i(\underline{r}) = \epsilon_i \varphi_i(\underline{r})$$

$$v_{\text{eff}}(\underline{r}) = v_{\text{ext}}(\underline{r}) + e^2 \int \frac{n(\underline{r}')}{|\underline{r} - \underline{r}'|} d\underline{r}' + \frac{\delta E_{\text{xc}}[n]}{\delta n}(\underline{r})$$

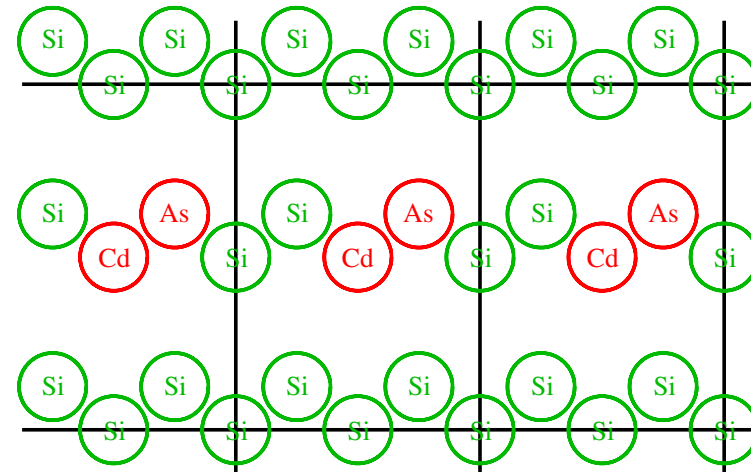
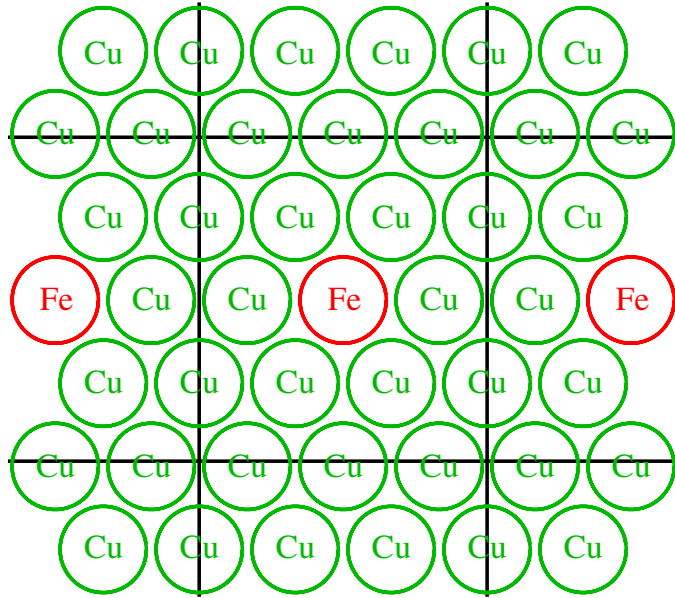
solution methods for non-periodic materials needed

Supercell techniques



potential and density essentially change in the vicinity of the defect atoms

Supercell techniques

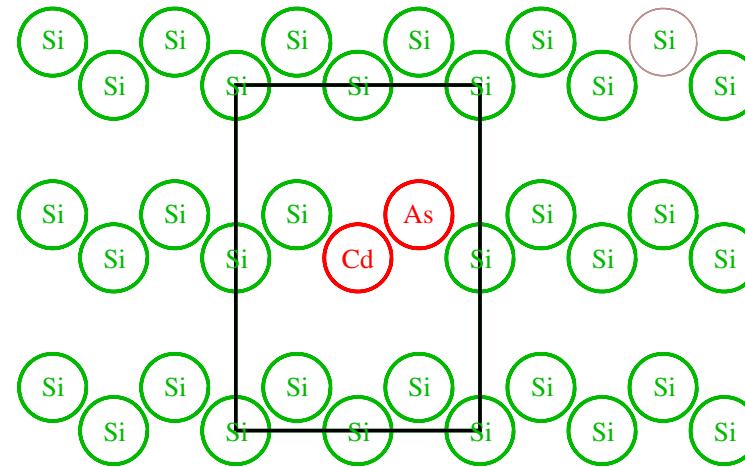
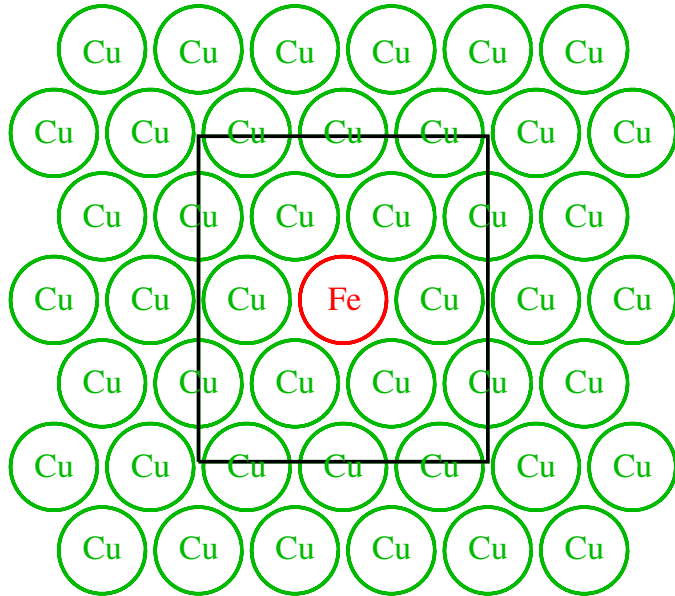


advantage: well tested computer codes for periodic systems can be used

disadvantage: spurious interactions between defect atoms are introduced

vacancy in Si: Puska et al. (1998), Corsetti et al. (2011)

Green function techniques



advantage: no spurious defect interactions

disadvantage: difficult development of computer codes

Green functions

- Laplace equation

$$\nabla_{\underline{r}}^2 G(\underline{r}, \underline{r}', 0) = \delta(\underline{r} - \underline{r}')$$

- Helmholtz equation

$$[-\nabla_{\underline{r}}^2 - \epsilon]G(\underline{r}, \underline{r}', \epsilon) = -\delta(\underline{r} - \underline{r}')$$

- Poisson equation

$$\nabla_{\underline{r}}^2 v(\underline{r}) = -4\pi n(\underline{r}) \Rightarrow v(\underline{r}) = \int d\underline{r}' \frac{1}{|\underline{r} - \underline{r}'|} n(\underline{r}')$$

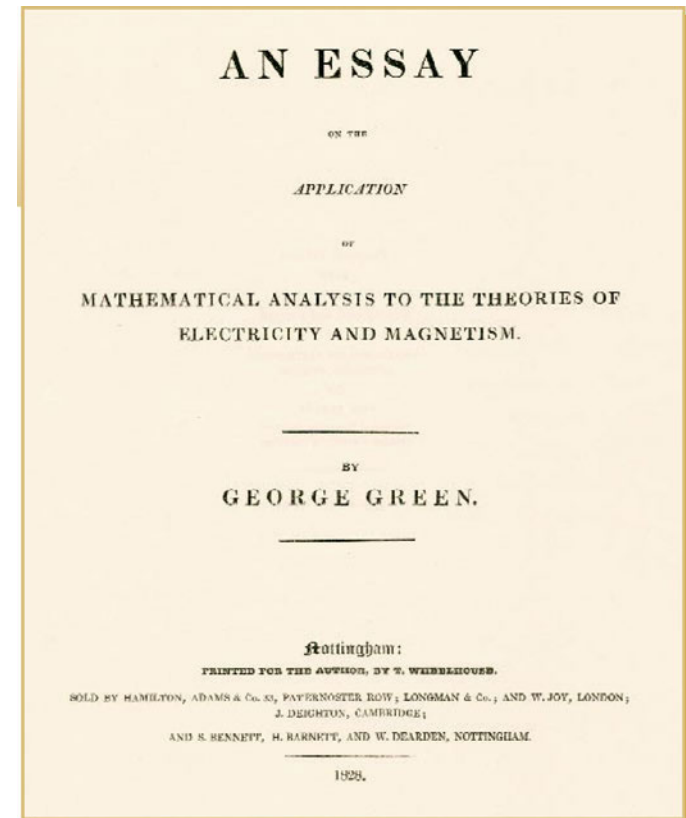
- Schroedinger equation

$$[-\nabla_{\underline{r}}^2 - \epsilon_i]\varphi_i(\underline{r}) = -v_{\text{eff}}(\underline{r})\varphi_i(\underline{r})$$

$$\Rightarrow \varphi_i(\underline{r}) = \int d\underline{r}' G(\underline{r}, \underline{r}', \epsilon_i) v_{\text{eff}}(\underline{r}') \varphi_i(\underline{r}')$$

$$G(\underline{r}, \underline{r}', \epsilon) = -\frac{1}{4\pi} \frac{\exp(i\sqrt{\epsilon}|\underline{r} - \underline{r}'|)}{|\underline{r} - \underline{r}'|}$$

George Green (1793-1841)



Green function properties

- spectral representation

$$\mathcal{H}\varphi_i(\underline{r}) = [-\nabla_{\underline{r}}^2 + v_{\text{eff}}(\underline{r})]\varphi_i(\underline{r}) = \epsilon_i\varphi_i(\underline{r})$$

$$[\mathcal{H} - \epsilon]G(\underline{r}, \underline{r}'; \epsilon) = [-\nabla_{\underline{r}}^2 + v_{\text{eff}}(\underline{r}) - \epsilon]G(\underline{r}, \underline{r}'; \epsilon) = -\delta(\underline{r} - \underline{r}')$$

operator notation $[\mathcal{H} - \epsilon]G = -I \Rightarrow G = \frac{1}{\epsilon - \mathcal{H}}$

representations in terms of eigenvalues and eigenvectors

$$\mathcal{H} = \sum_i \epsilon_i \varphi_i(\underline{r}) \varphi_i^*(\underline{r}') \Rightarrow G = \sum_i \frac{1}{\epsilon - \epsilon_i} \varphi_i(\underline{r}) \varphi_i^*(\underline{r}')$$

Green function properties

- **analytical properties** $G(\underline{r}, \underline{r}'; \epsilon) = \sum_i \frac{1}{\epsilon - \epsilon_i} \varphi_i(\underline{r}) \varphi_i^*(\underline{r}')$

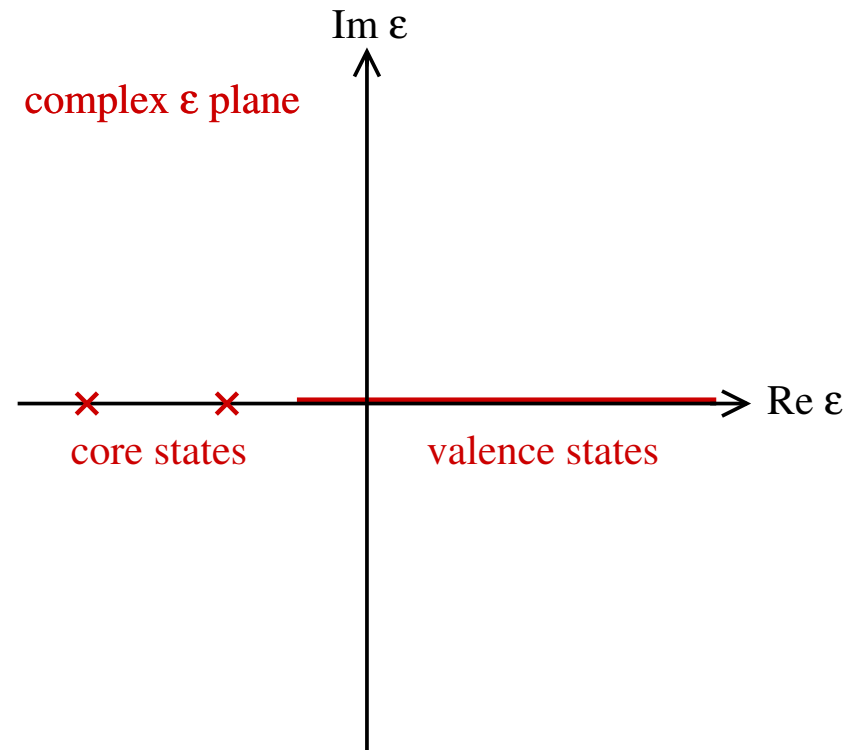
poles for real values $\epsilon = \epsilon_i$

branch cuts for real values ϵ

elsewhere infinitely differentiable

\Rightarrow analytic in complex plane

discrete and **continuous** parts
of the eigenvalue spectrum



Green function properties

• **connection with density** $G(\underline{r}, \underline{r}; \epsilon) = \sum_i \frac{1}{\epsilon - \epsilon_i} \varphi_i(\underline{r}) \varphi_i^*(\underline{r})$

$$n(\underline{r}) = 2 \sum_i \varphi_i(\underline{r}) \varphi_i^*(\underline{r}) = 2 \int_{-\infty}^{E_F} d\epsilon \delta(\epsilon - \epsilon_i) \varphi_i(\underline{r}) \varphi_i^*(\underline{r})$$

$$\pi \delta(\epsilon - \epsilon_i) = \lim_{\gamma \rightarrow 0^+} \frac{\gamma}{(\epsilon - \epsilon_i)^2 + \gamma^2} = - \lim_{\gamma \rightarrow 0^+} \text{Im} \frac{1}{\epsilon - \epsilon_i + i\gamma}$$

$$n(\underline{r}) = -\frac{2}{\pi} \lim_{\gamma \rightarrow 0^+} \int_{-\infty}^{E_F} d\epsilon \text{Im} G(\underline{r}, \underline{r}; \epsilon + i\gamma)$$

- **connection with density of states**

$$n_V(\epsilon) = \int_V d\underline{r} \sum_i \delta(\epsilon - \epsilon_i) \varphi_i(\underline{r}) \varphi_i^*(\underline{r}) = -\frac{2}{\pi} \int_V d\underline{r} \text{Im} G(\underline{r}, \underline{r}; \epsilon)$$

Complex energy integration

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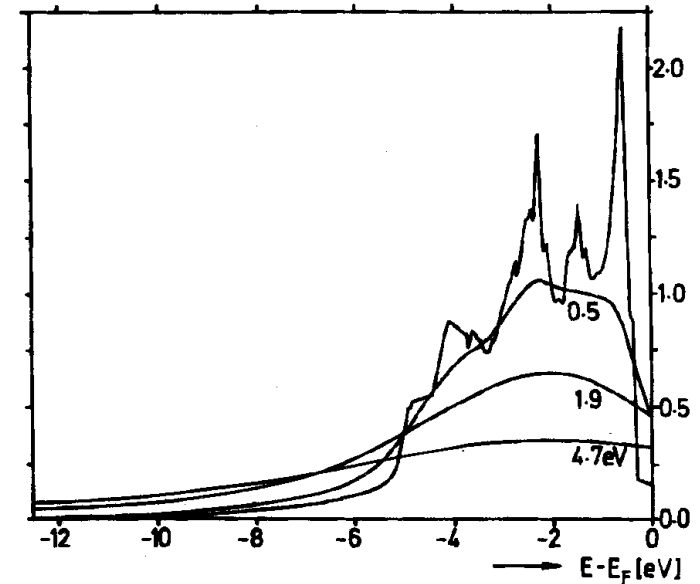
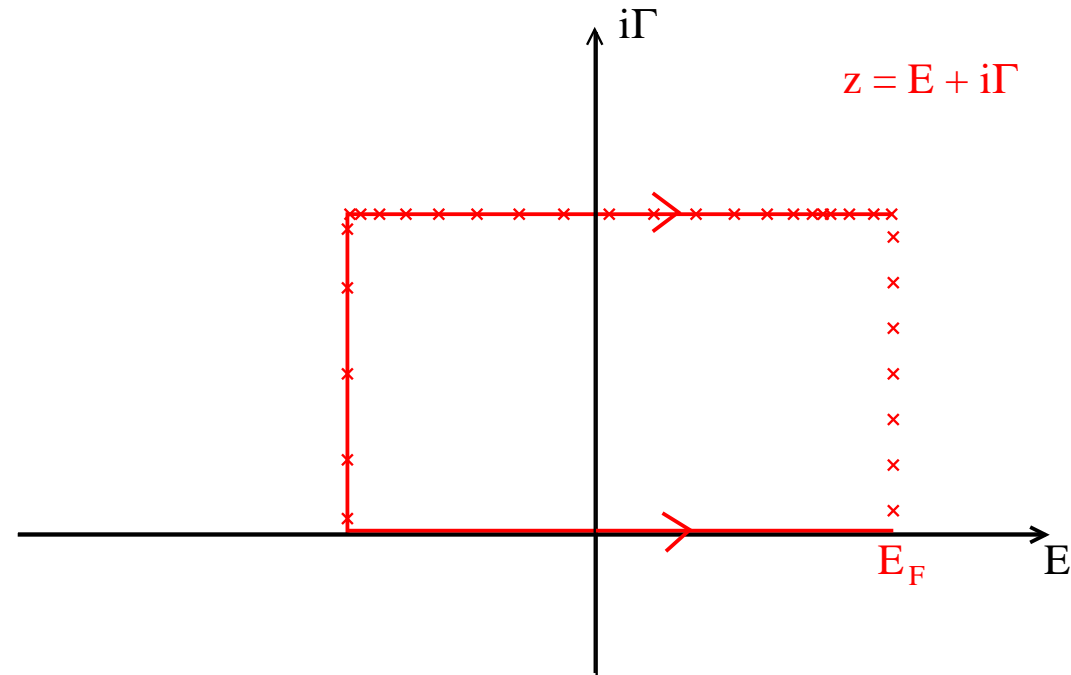


Fig. 2: a) Density of states for the majority electrons of Ni and the corresponding quantity along paths parallel to the real axis for various distances $\Gamma=0.5, 1.9$ and 4.7 eV.

Solid State Comm. (1982)

$$\begin{aligned}
 n(\underline{r}) &= -\frac{2}{\pi} \text{Im} \int_{-\infty}^{\infty} d\epsilon G(\underline{r}, \underline{r}, \epsilon) f(\epsilon, T) \\
 &= -\frac{2}{\pi} \text{Im} \sum_j w_j G(\underline{r}, \underline{r}, \epsilon_j)
 \end{aligned}$$

complex analysis: residue theorem

Fermi-Dirac function $f(\epsilon, T)$

\Rightarrow about 30 mesh points ϵ_j are enough

Concept of reference systems

instead of differential equation use integral equation

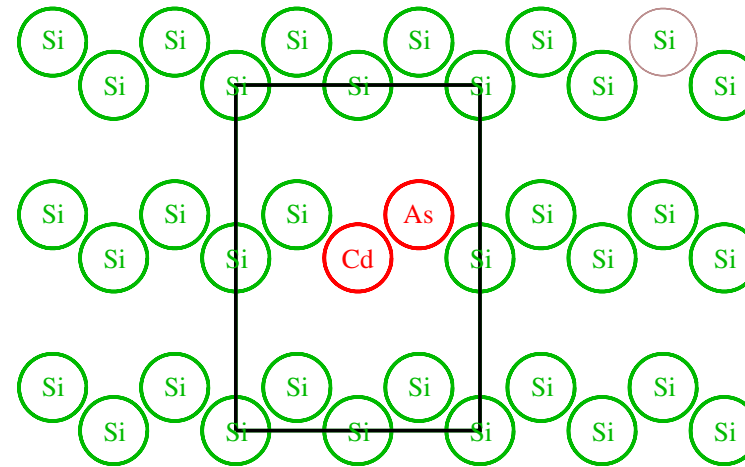
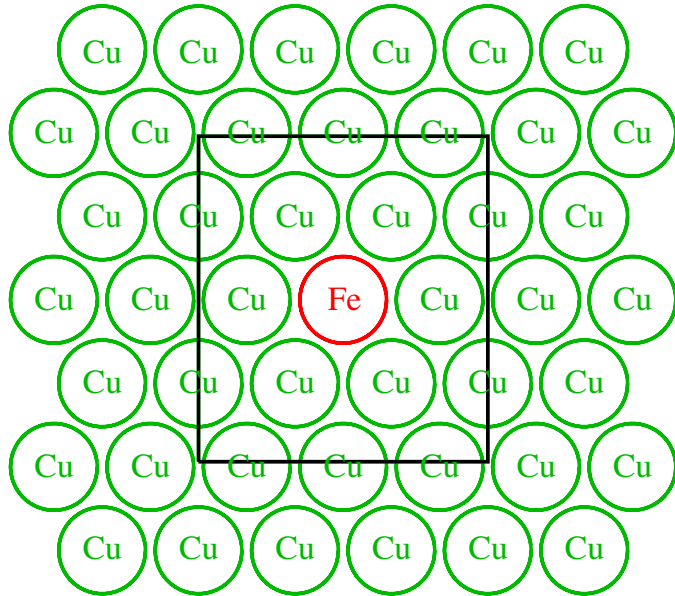
$$G(\underline{r}, \underline{r}'; \epsilon) = G^r(\underline{r}, \underline{r}'; \epsilon) + \int d\underline{r}'' G^r(\underline{r}, \underline{r}''; \epsilon) [v_{\text{eff}}(\underline{r}'') - v^r(\underline{r}'')] G(\underline{r}'', \underline{r}'; \epsilon)$$

with known **Green function** G^r of a suitably chosen reference system

$$\left[-\nabla_{\underline{r}}^2 + v^r(\underline{r}) - \epsilon \right] G^r(\underline{r}, \underline{r}'; \epsilon) = -\delta(\underline{r} - \underline{r}')$$

use **unperturbed host Green function** to calculate **impurity Green function**

Green function techniques



advantage: no spurious defect interactions

disadvantage: difficult development of computer codes

Green function for periodic systems

History

- Wannier functions (Koster, Slater 1954)
- LCAO (Baraff, Schlüter 1978; Bernholc, Lipari, Pantelides 1978)
- LCGO (Singhal, Callaway 1979)
- KKR (Zeller, Dederichs 1979)
- LMTO (Gunnarsson, Jepsen, Andersen 1983)

calculation by spectral representation and Kramers-Kronig relation

$$\operatorname{Re}G(\underline{r}, \underline{r}'; \epsilon) = -\frac{1}{\pi}P \int_{-\infty}^{\infty} d\epsilon' \frac{1}{\epsilon - \epsilon'} \operatorname{Im}G(\underline{r}, \underline{r}'; \epsilon')$$

Green function of a complicated system

$$G = G^r + G^r [V - V^r] G$$

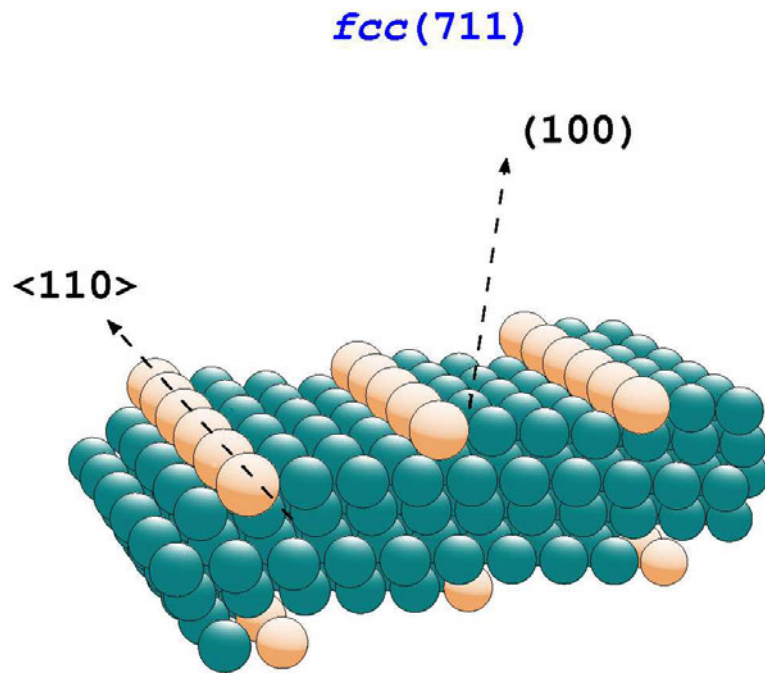
by successive calculation of Green functions of simpler systems

1. free space \Rightarrow ideal crystal
2. ideal crystal \Rightarrow crystal with surface
3. crystal with surface \Rightarrow adsorbate atoms

Advantages

1. the region, where the potential changes, is exactly embedded in a simpler system
2. integral equation is restricted in space to the region, where the potential changes
3. all interactions, e.g., between adsorbed clusters and the substrate are included

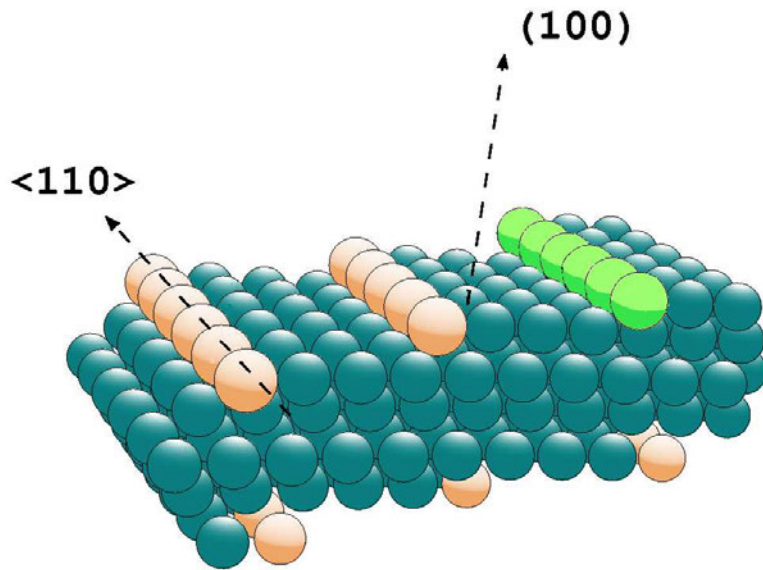
Example: vicinal surface with nanowires



1. Green function of free space
2. periodic bulk system
three-dimensional periodicity
3. surface construction (empty layers)
two-dimensional periodicity

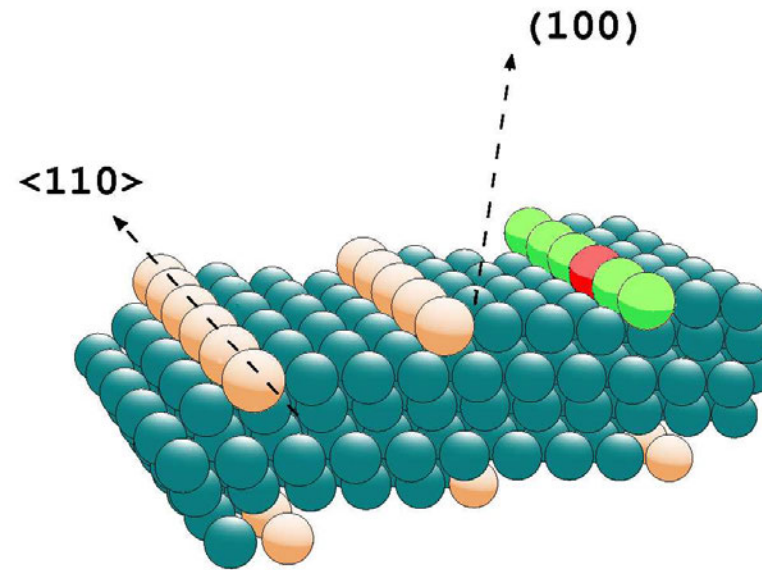
Further examples

fcc(711)



atomic chains
one-dimensional periodicity

fcc(711)

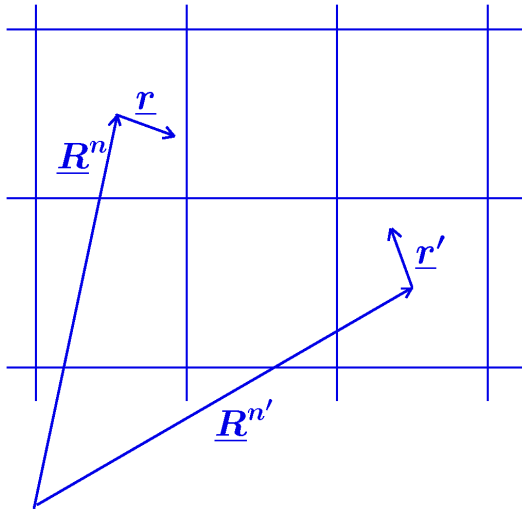


adsorbate atoms
real space calculation

modern DFT-GF techniques: LMT0 and KKR methods

KKR Green function method

$$G(\underline{r} + \underline{R}^n, \underline{r}' + \underline{R}^{n'}) = \delta^{nn'} G_s^n(\underline{r}, \underline{r}') + \sum_{LL'} R_L^n(\underline{r}) G_{LL'}^{nn'} R_{L'}^{n'}(\underline{r}')$$



- **divide space into cells n**
- **solve single-cell problems**

$$G_s^n(\underline{r}, \underline{r}') = G^0(\underline{r}, \underline{r}') + \int_n d\underline{r}'' G^0(\underline{r}, \underline{r}'') V(\underline{r}'') G_s^n(\underline{r}'', \underline{r}')$$

$$R_L^n(\underline{r}) = J_L(\underline{r}) + \int_n d\underline{r}' G^0(\underline{r}, \underline{r}') V(\underline{r}') R_L^n(\underline{r}')$$

- **use matrix equation**

$$G_{LL'}^{nn'} = G_{LL'}^{r,nn'} + \sum_{n''L''L'''} G_{LL''}^{r,nn''} \Delta t_{L''L'''}^{n''} G_{L'''L'}^{n''n'}$$

$$\Delta t_{LL'}^n = \int_n d\underline{r} R_L^{r,n}(\underline{r}) \Delta V(\underline{r}) R_{L'}^n(\underline{r})$$

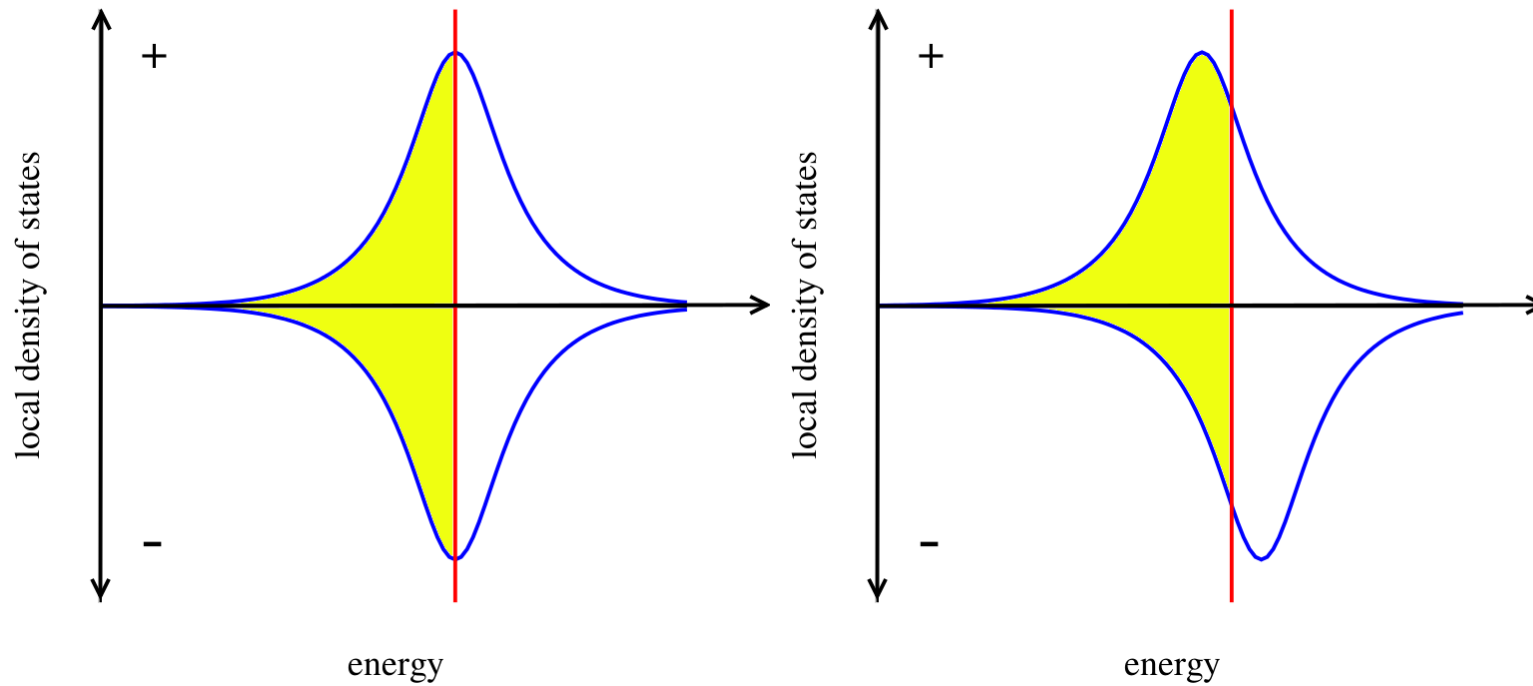
single-cell integral equations

matrix equation does not depend on radial resolution

angular variables lead to L, L' indices (usually 16 or 25 enough)

Friedel-Anderson virtual bound state model

discrete atomic d states hybridize with conduction states



$$M = \int_{-\infty}^{E_F} d\epsilon [n^+(\epsilon) - n^-(\epsilon)]$$

splitting $\sim M$

Friedel-Anderson virtual bound state model

KKR-GF calculations (Z. Phys 1980)

experiment

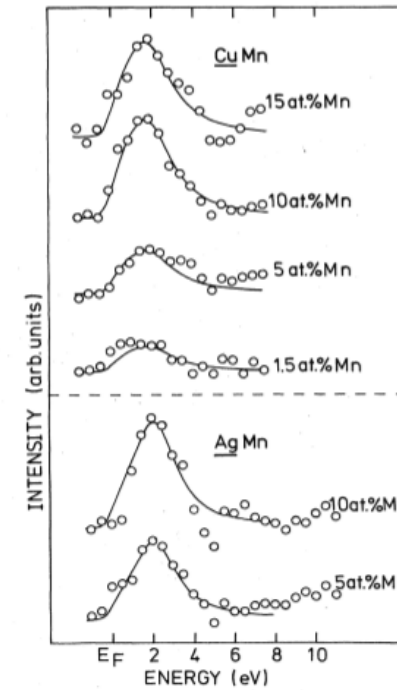
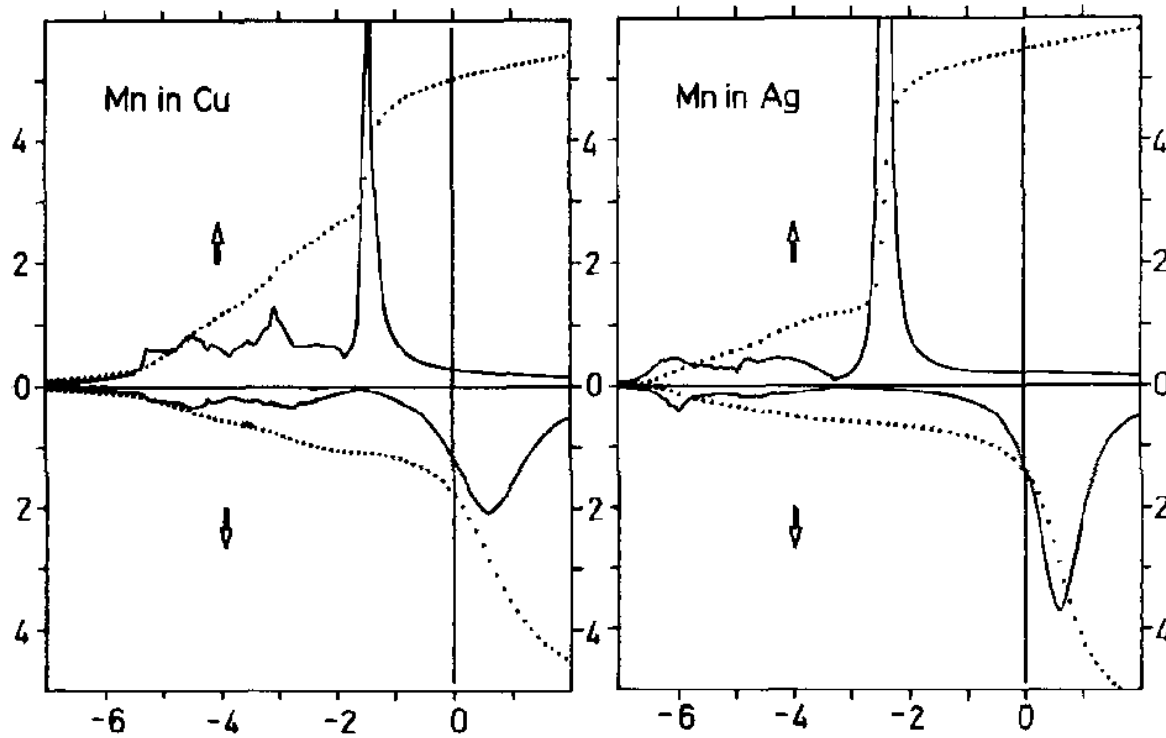


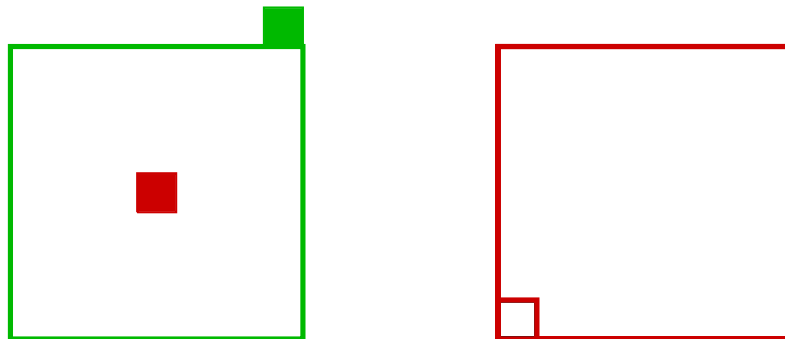
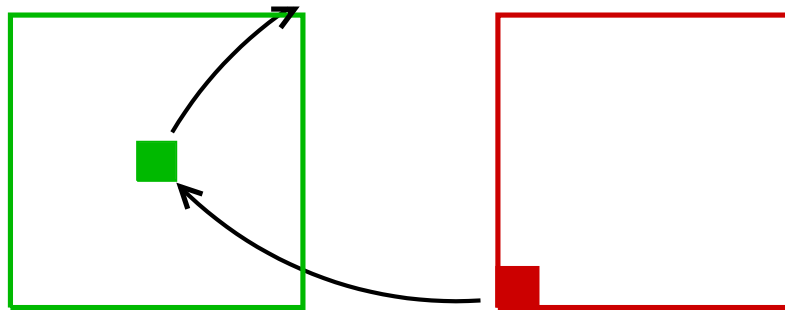
FIG. 11. Difference spectra of the AgMn and CuMn BIS spectra and the corresponding pure-metal spectra.

van der Marel et al.
Phys. Rev. B (1985)

Solution energies

crystal A

crystal B



- $E_s^{\text{B in A}} = \Delta E_{\text{BA}} - E_{\text{A}} + E_{\text{B}}$

- typical values for E and ΔE

$$E_{\text{A,B}} = 10^4 - 10^6 \text{ eV}$$

$$E_s = 10^{-2} - 10^0 \text{ eV}$$

\Rightarrow high precision is required

- modified energy functional

$$\tilde{E}[n(\underline{r})] = E[n(\underline{r})]$$

$$- E_F \left(\int d\underline{r} n(\underline{r}) - N \right)$$

Phys. Rev. B (1989)

Formation and solution energies

vacancy formation energy (in eV)

	Cu	Ag	Ni	Pd
Theory	1.37	1.20	1.68	1.57
Experiment	1.28	1.11	1.79, 1.63	1.85, 1.54

solution energy (in eV) for V in Cu

shells	0	1	2	3	4
cells	1	13	19	43	55
E_{Lloyd}	1.44	0.73	0.73	0.73	0.73
E_{local}	1.60	1.93	1.38	0.75	0.52

(Solid State Comm. 1991)

relaxation energy for Cu and Ni included

-0.04 eV and -0.08eV

(Phys. Rev B 1989)

importance of Lloyd's formula

single-particle energies $E_{\text{sp}} = \int_{-\infty}^{E_F} d\epsilon \epsilon n(\epsilon)$

integration over all space

Solution energies

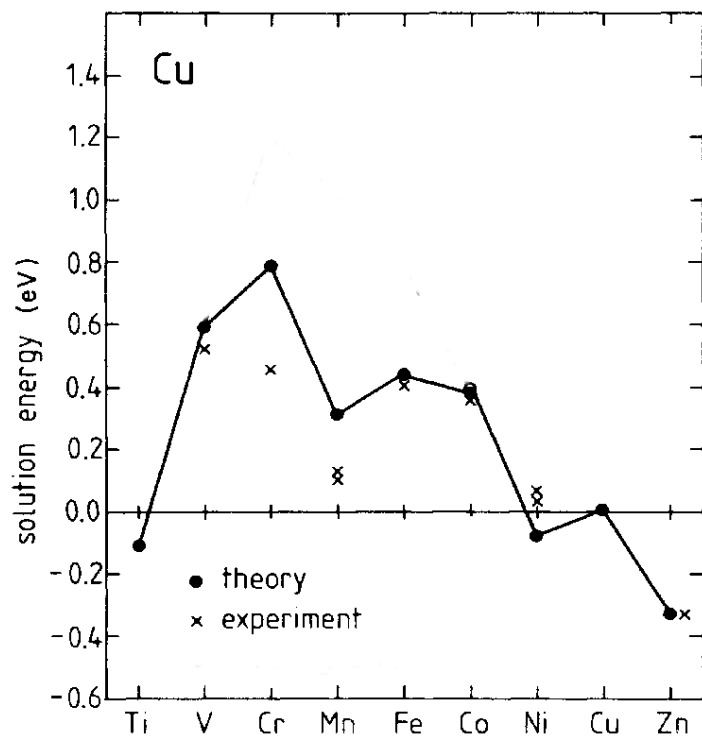


FIG. 1. Solution energies of 3d impurities in Cu

endothermic solubility

Phys. Rev. B (1989)

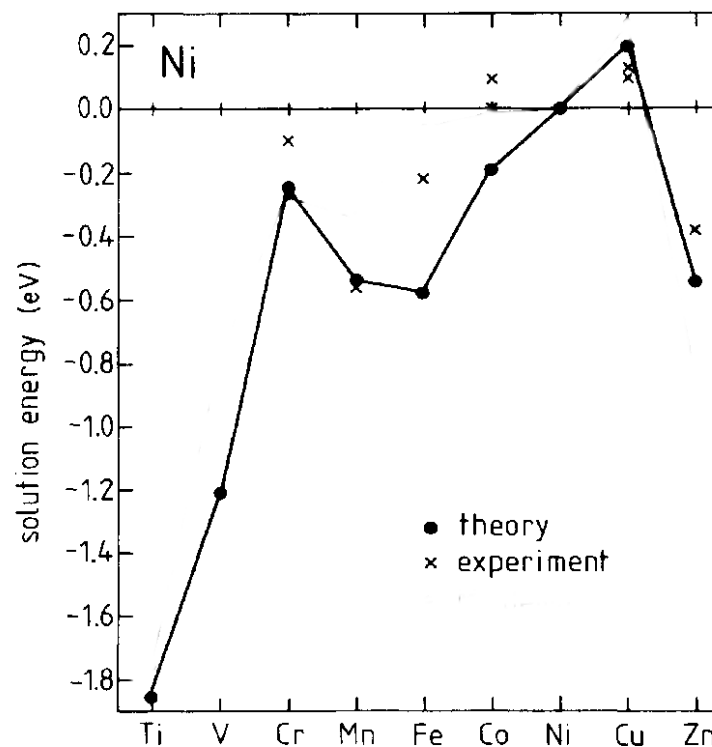
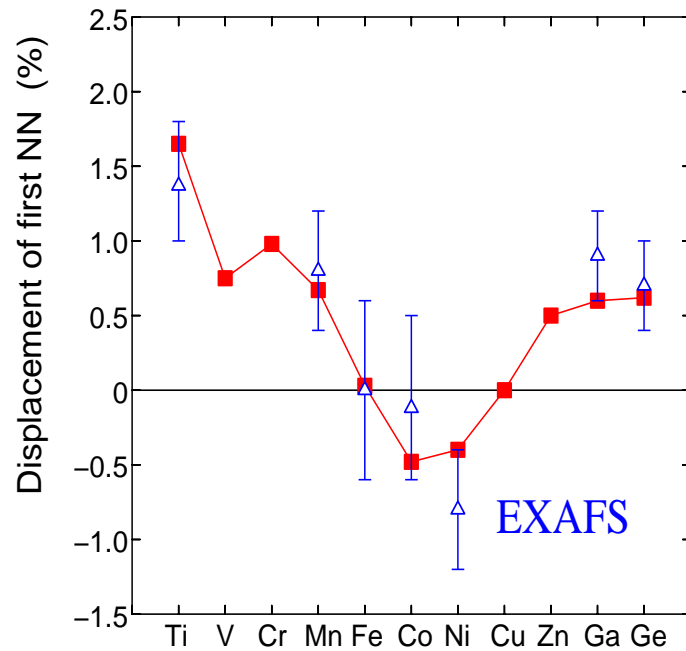


FIG. 2. Solution energies of 3d impurities in Ni

exothermic solubility

Forces and relaxations



displacement of nearest Cu neighbour atoms around impurities

Phys. Rev. B (1997)

for forces: **Hellmann-Feynman theorem**

$$\mathcal{H}(\lambda) |\Psi_i(\lambda)\rangle = E_i |\Psi_i(\lambda)\rangle$$

orthonormal eigenfunctions

$$\langle \Psi_i(\lambda) | \Psi_j(\lambda) \rangle = \delta_{ij}$$

$$\left\langle \frac{\partial \Psi_i(\lambda)}{\partial \lambda} | \Psi_j(\lambda) \right\rangle = 0$$

$$E_i(\lambda) = \langle \Psi_i(\lambda) | \mathcal{H}(\lambda) | \Psi_i(\lambda) \rangle$$

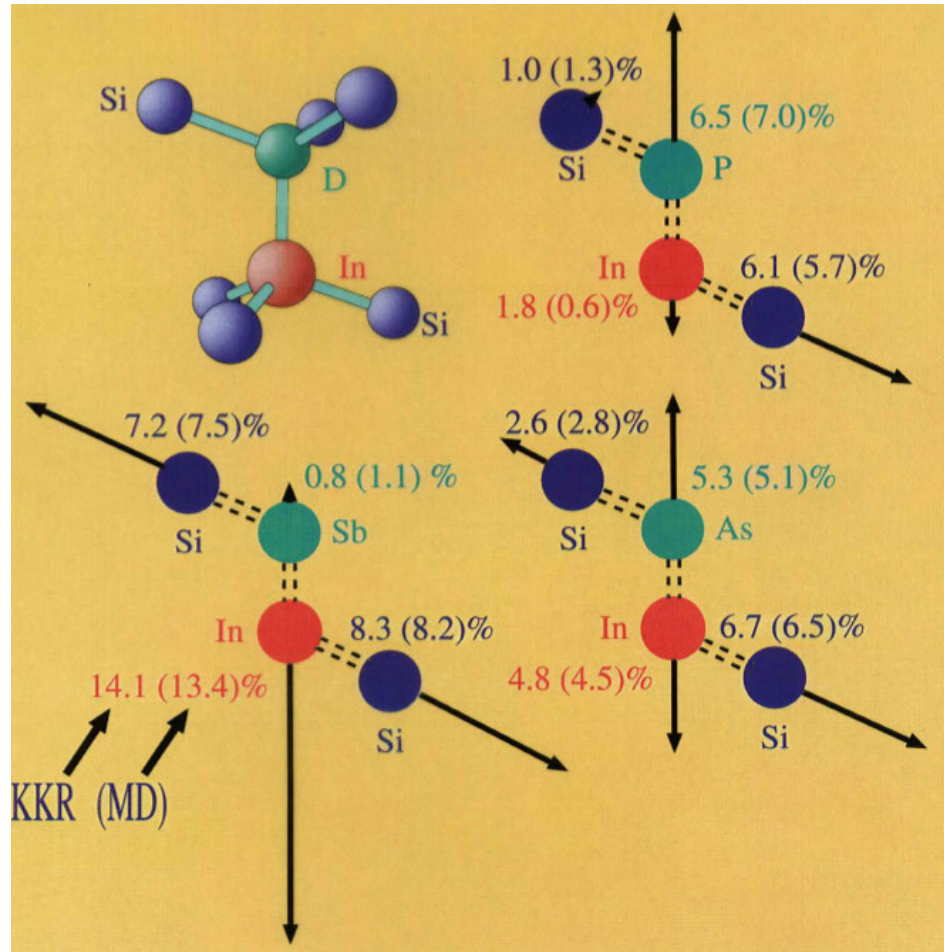
$$\frac{\partial E_i(\lambda)}{\partial \lambda} = \left\langle \Psi_i(\lambda) \left| \frac{\partial \mathcal{H}(\lambda)}{\partial \lambda} \right| \Psi_i(\lambda) \right\rangle$$

$$\mathbf{F}^n = - \frac{\partial E}{\partial \mathbf{R}^n} \Big|_{n(\mathbf{r}; \mathbf{R}^n)} - \int d\mathbf{r} \frac{\delta E}{\delta n(\mathbf{r})} \frac{\partial n(\mathbf{r}; \mathbf{R}^n)}{\partial \mathbf{R}^n}$$

$$\mathbf{F}^n = Z^n \frac{\partial V_M(\mathbf{r})}{\partial \mathbf{r}} \Big|_{\mathbf{r}=\mathbf{R}^n} - \int d^3r n_{\text{core}}(|\mathbf{r}-\mathbf{R}^n|) \frac{\partial v_{\text{eff}}(\mathbf{r})}{\partial \mathbf{r}}$$

for displacements: **U transformation**

Indium-donor complexes in Si



electric field gradient

calc.: $l = 2$ components of $V_{\text{Coul}}^n(\underline{r} = 0)$

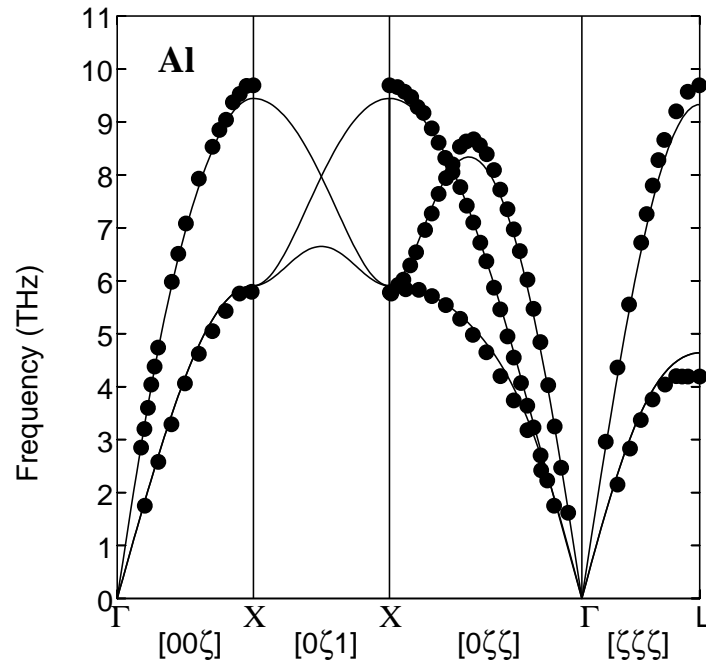
exp.: nuclear quadrupole constant ν

TABLE I. The quadrupole coupling constant at the Cd site, $\nu = eQ_{\text{Cd}}V_{zz}/h$, calculated using a nuclear quadrupole moment $Q_{\text{Cd}} = 0.83$ b and the largest component, V_{zz} , of the EFG tensor.

	EFG _{ideal}	EFG _{relaxed}	EFG _{exp} [1–5]
	Si host		
$[\text{CdP}]^-$	-189	-191	± 179
$[\text{CdAs}]^-$	-174	-249	± 229
$[\text{CdSb}]^-$	-85	-294	± 271
$[\text{CdP}]^0$	-79	-56	± 36
$[\text{CdAs}]^0$	-73	-89	± 83
$[\text{CdSb}]^0$	+6	-135	± 129

Phys. Rev. Lett. (1999)

Phonons



- displace central Al atom by 0.5 %
- calculate forces on six shells of neighbours
⇒ Born-von Karman force constants
- Fourier transform force constant matrix
- determine eigenvalues of dynamical matrix
⇒ phonon frequencies

phonons are usually calculated with supercell techniques
Green function calculations [Phys. Rev. B \(1998\)](#)

Long range perturbations

Friedel oscillations

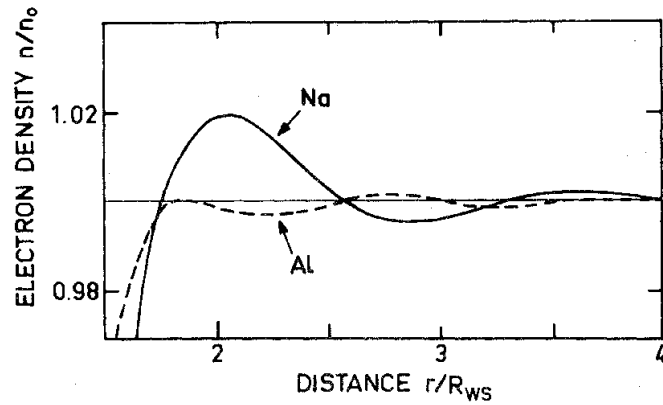


FIG. 3. The first Friedel oscillations in electron densities at vacancies of sodium and aluminum.

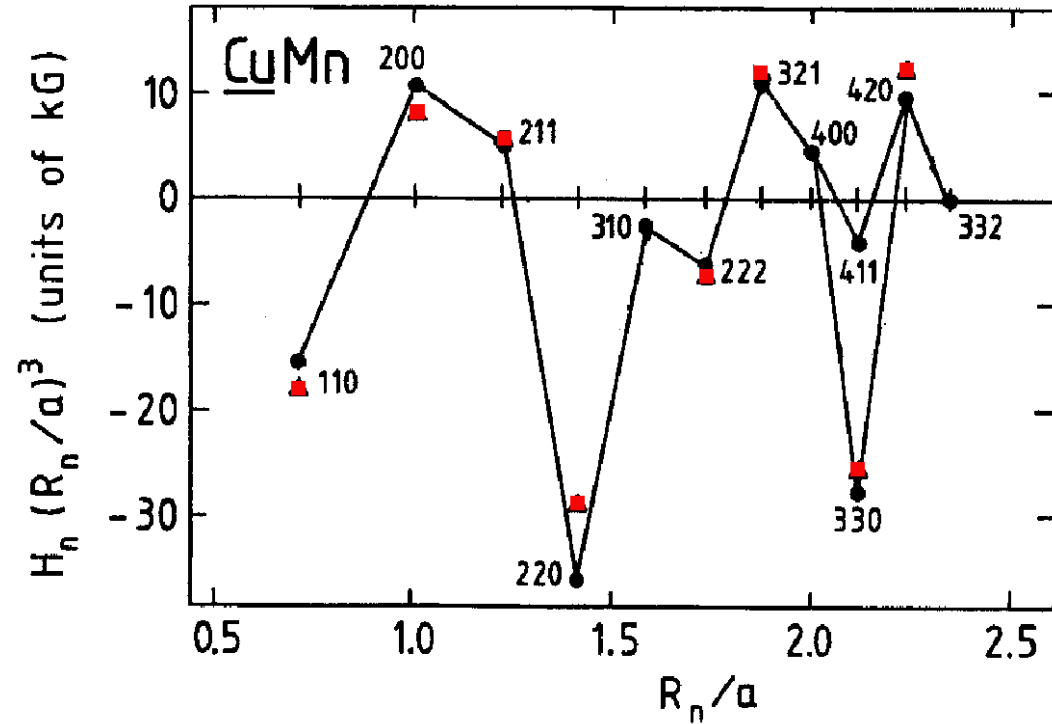
Manninen et al., Phys. Rev. B (1975)

nuclear magnetic resonance
Knight shift of frequencies

hyperfine field

$$H_f^n = \frac{8\pi}{3} \mu_B [n^+(\underline{R}^n) - n^-(\underline{R}^n)]$$

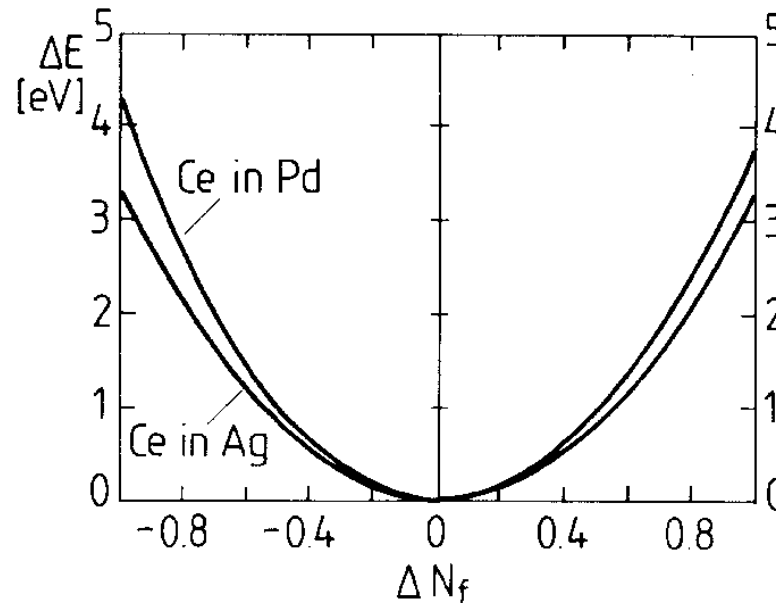
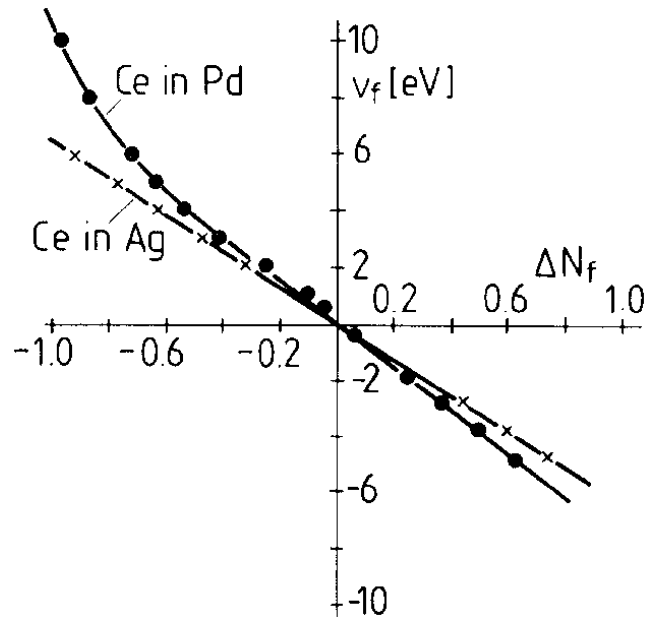
comparison experiment and GF calculation



Phys. Rev. B (1989)

Constrained density functional theory

useful to calculate parameters for model Hamiltonians *Phys. Rev. Lett.* (1984)



modified energy functional

Hellmann-Feynman theorem

Coulomb parameters (Hubbard U)

$$\tilde{E}[n(\underline{r})] = E[n(\underline{r})] + v_f \left[N_f - \int_V n_f(\underline{r}) d\underline{r} \right]$$

$$\frac{d\tilde{E}(N_f)}{dN_f} = v_f \quad \Rightarrow \quad \Delta\tilde{E}(N_f) = \int_{N_f^0}^{N_f} v_f(N') dN'$$

$$U_f = \Delta E(N_f^0 + 1) + \Delta E(N_f^0 - 1)$$

Constrained Density Functional Theory

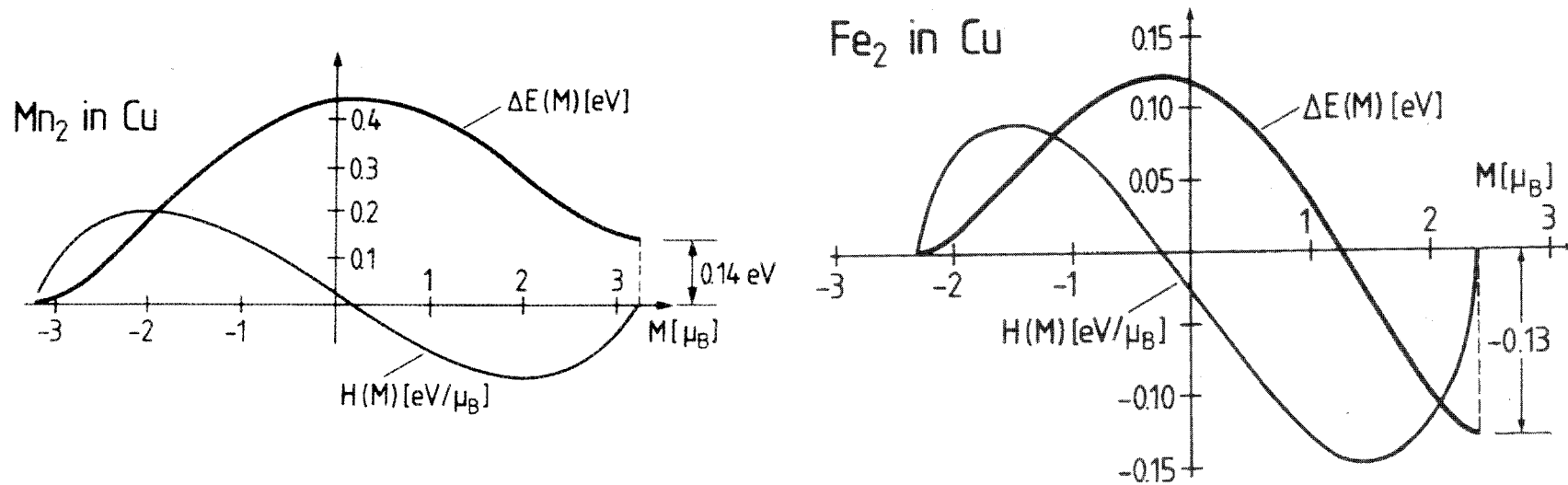
interaction of magnetic impurities



$$\tilde{E}[n(\underline{r}), m(\underline{r})] = E[n(\underline{r}), m(\underline{r})] + H \left[\mu_B M - \int_{V_1} m(\underline{r}) d\underline{r} \right]$$

$$\Delta E(M) = \int_{M_0}^M H(M') dM'$$

Interaction of Magnetic Impurities in Cu



mapping to Heisenberg model

$$\Delta E(\underline{M}_i, \underline{M}_j) \approx -\frac{1}{2} \sum_{i,j} \sum J_{ij} \Delta \underline{M}_i \Delta \underline{M}_j$$

J. Magn. Magn. Mat. (1986)

Random alloys

important quantity: single-site operator $t_\alpha = V_\alpha + V_\alpha g t_\alpha$ ($V = \sum_\alpha V_\alpha$)

$$t_\alpha(\underline{r}, \underline{r}') = V_\alpha(\underline{r})\delta(\underline{r} - \underline{r}') + \int d\underline{r}'' V_\alpha(\underline{r})g(\underline{r}, \underline{r}'')t_\alpha(\underline{r}'', \underline{r}')$$

equation for averaged Green function $\langle G \rangle$ is needed formally $G = F \langle G \rangle$

$$G = g + gVG$$

$$F \langle G \rangle = g + gVF \langle G \rangle$$

average

$$\langle G \rangle = g + g \langle VF \rangle \langle G \rangle$$

here V depends on the complicated statistical contribution of V_α
whereas the **self-energy** $\Sigma = \langle VF \rangle$ is an averaged quantity

Random alloys

introduce single-site operators f_α by the condition $V_\alpha F = t_\alpha f_\alpha$

$\Rightarrow \Sigma = \langle VF \rangle = \sum_\alpha \langle t_\alpha f_\alpha \rangle$ and equation for f_α

$$f_\alpha = 1 + \sum_{\beta \neq \alpha} g t_\beta f_\beta - \sum_{\beta} g \langle t_\beta f_\beta \rangle$$

$$f_\alpha = 1 + \sum_{\beta \neq \alpha} g t_\beta - \sum_{\beta} g \langle t_\beta \rangle \dots \quad \text{by iteration}$$

$$f_\alpha = 1 + \sum_{\beta \neq \alpha} \beta - \sum_{\beta} \langle \beta \rangle \dots \quad \text{in simpler notation}$$

$$\langle t_\alpha f_\alpha \rangle = \langle \alpha \rangle + \sum_{\beta \neq \alpha} \langle \alpha \beta \rangle - \sum_{\beta} \langle \alpha \rangle \langle \beta \rangle \dots$$

Random alloys: approximations

$$\begin{aligned}
 \langle VF \rangle &= \sum_{\alpha} \langle t_{\alpha} f_{\alpha} \rangle = \sum_{\alpha} \langle \alpha \rangle \\
 &+ \sum_{\alpha} \sum_{\beta \neq \alpha} \langle \alpha \beta \rangle - \sum_{\alpha} \sum_{\beta} \langle \alpha \rangle \langle \beta \rangle \\
 &+ \sum_{\alpha} \sum_{\beta \neq \alpha} \sum_{\gamma \neq \beta} \langle \alpha \beta \gamma \rangle - \sum_{\alpha} \sum_{\beta \neq \alpha} \sum_{\gamma} \langle \alpha \beta \rangle \langle \gamma \rangle \\
 &- \sum_{\alpha} \sum_{\beta} \sum_{\gamma \neq \beta} \langle \alpha \rangle \langle \beta \gamma \rangle + \sum_{\alpha} \sum_{\beta} \sum_{\gamma} \langle \alpha \rangle \langle \beta \rangle \langle \gamma \rangle + \dots
 \end{aligned}$$

no correlations: $\langle \alpha \beta \rangle = (1 - \delta_{\alpha \beta}) \langle \alpha \rangle \langle \beta \rangle + \delta_{\alpha \beta} \langle \alpha \alpha \rangle$

$$\begin{aligned}
 \langle VF \rangle &= \sum_{\alpha} \langle t_{\alpha} f_{\alpha} \rangle = \sum_{\alpha} \langle \alpha \rangle - \sum_{\alpha} \langle \alpha \rangle \langle \alpha \rangle \\
 &+ \sum_{\alpha} \langle \alpha \rangle \langle \alpha \rangle \langle \alpha \rangle + \sum_{\alpha} \sum_{\beta \neq \alpha} \langle \alpha \rangle \langle \beta \rangle \langle \alpha \rangle - \sum_{\alpha} \sum_{\beta \neq \alpha} \langle \alpha \rangle \langle \beta \rangle \langle \alpha \rangle - \dots
 \end{aligned}$$

in 4th order $\langle \alpha \beta \gamma \delta \rangle$ leads to complicated term $\langle {}_a \alpha \langle {}_b \beta \alpha \rangle_a \beta \rangle_b$

Random alloys: approximation

$$\begin{aligned} \Sigma = \langle VF \rangle &= \sum_{\alpha} \langle t_{\alpha} f_{\alpha} \rangle = \sum_{\alpha} \langle \alpha \rangle - \sum_{\alpha} \langle \alpha \rangle \langle \alpha \rangle \\ &+ \sum_{\alpha} \langle \alpha \rangle \langle \alpha \rangle \langle \alpha \rangle + \sum_{\alpha} \sum_{\beta \neq \alpha} \langle \alpha \rangle \langle \beta \rangle \langle \alpha \rangle - \sum_{\alpha} \sum_{\beta \neq \alpha} \langle \alpha \rangle \langle \beta \rangle \langle \alpha \rangle - \dots \end{aligned}$$

virtual crystal approximation (VCA) $F = 1 \Rightarrow \langle VF \rangle = \sum_{\alpha} \langle V_{\alpha} \rangle$

average t matrix approximation (ATA) $\Sigma = \sum_{\alpha} \langle \alpha \rangle$

method of optical potential $\Sigma = \sum_{\alpha} \langle \alpha \rangle - \sum_{\alpha} \langle \alpha \rangle \langle \alpha \rangle + \sum_{\alpha} \langle \alpha \rangle \langle \alpha \rangle \langle \alpha \rangle - \dots$

self-consistent approximation (CPA) choose g such that $\langle \alpha \rangle = \langle t_{\alpha} \rangle = 0$ **effective medium**

$t_{\alpha}(\underline{r}, \underline{r}')$ is a **non-local operator** \Rightarrow how to achieve $\langle t_{\alpha} \rangle = 0$

KKR-CPA: single-site t matrices, not dependent on spatial coordinates

Stocks et al. Phys. Rev. Lett. (1978), Bansil Phys. Rev. Lett. (1978)

Ferromagnetism of Alloys (Slater-Pauling curve)

ferromagnetic alloys

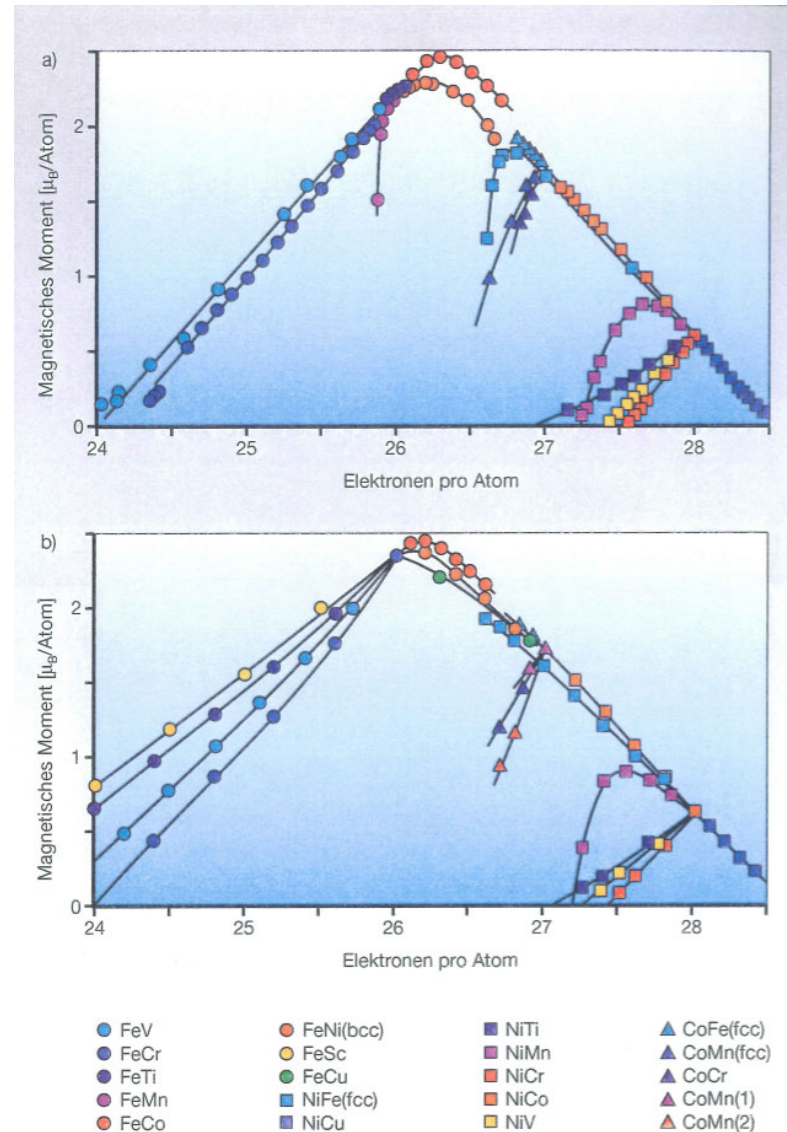
alloys of Fe, Co, Ni

also with other TM metals

systematic trends

KKR-CPA calculations

J. Magn. Magn. Mat. (1991)



Summary

- Introduction to GF methods
- Density of states
- Formation and solution energies
- Forces, displacements and phonons
- Long-range perturbations
- Constrained DFT
- Random alloys, KKR-CPA