LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

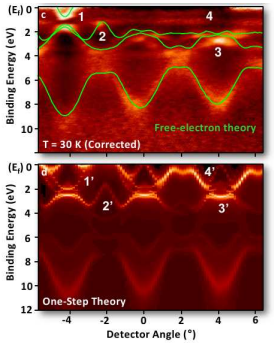
The Munich SPRKKR-program package
A spin polarised relativistic Korringa-Kohn-Rostoker code for calculating solid state properties

Ján Minár

H. Ebert, M. Battocletti, D. Benea, S. Bornemann, J. Braun, S. Chadov, M. Deng, H. Freyer, T. Huhne, M. Kardinal, D. Kodderitzsch, M. Kosuth, S. Lowitzer, S. Mankovskyy, M. Offenberger, A. Perlov, V. Popescu, Ch. Zecha and many others

Ludwig-Maximilians-Universität München, Germany

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{V} \hat{G}$$



Funding

Bundesministerium für Bildung und Forschung

DFG Deutsche Forschungsgemeinschaft

Outline

- Introduction
- Green's functions
- Scattering theory
- Angular momentum representation
- Calculating the scattering path operator
- The impurity problem
- Substitutationally disordered alloys
- Flow diagrams of SPR-KKR package
- Summary

More information on KKR

H. Ebert, D. Ködderitzsch and J. Minar

Calculating condensed matter properties using the KKR-Green's function method-recent developments and applications

Reports on Progress in Physics, **74**, 096501 (2011)

H. Ebert, et al.

Recent Developments in KKR Theory
Highlight of the Month" in: HCM - Newsletter of the ***k*** Network – ab initio (from electronic structure) calculation of complex processes in materials, **97**, 79 (2010)

http://www.kkr-gf.org/

Standard band structure approach I

- Born-Oppenheimer Approximation
- reduction of many-particle problem
  to single-particle problem
  e.g. via density functional theory (DFT)

$$\left[-\vec{\nabla}^2 + V(\vec{r})\right] \psi(\vec{r}, E) = E\psi(\vec{r}, E)$$

periodic potential $V(\vec{r}) = V(\vec{r} + \vec{R}_n)$

leads to the Bloch theorem

$$T_{\vec{R}_n} \psi_{\vec{k}}(\vec{r}, E) = e^{-i\vec{k}\vec{R}_n} \psi_{\vec{k}}(\vec{r}, E)$$

Standard band structure approach II

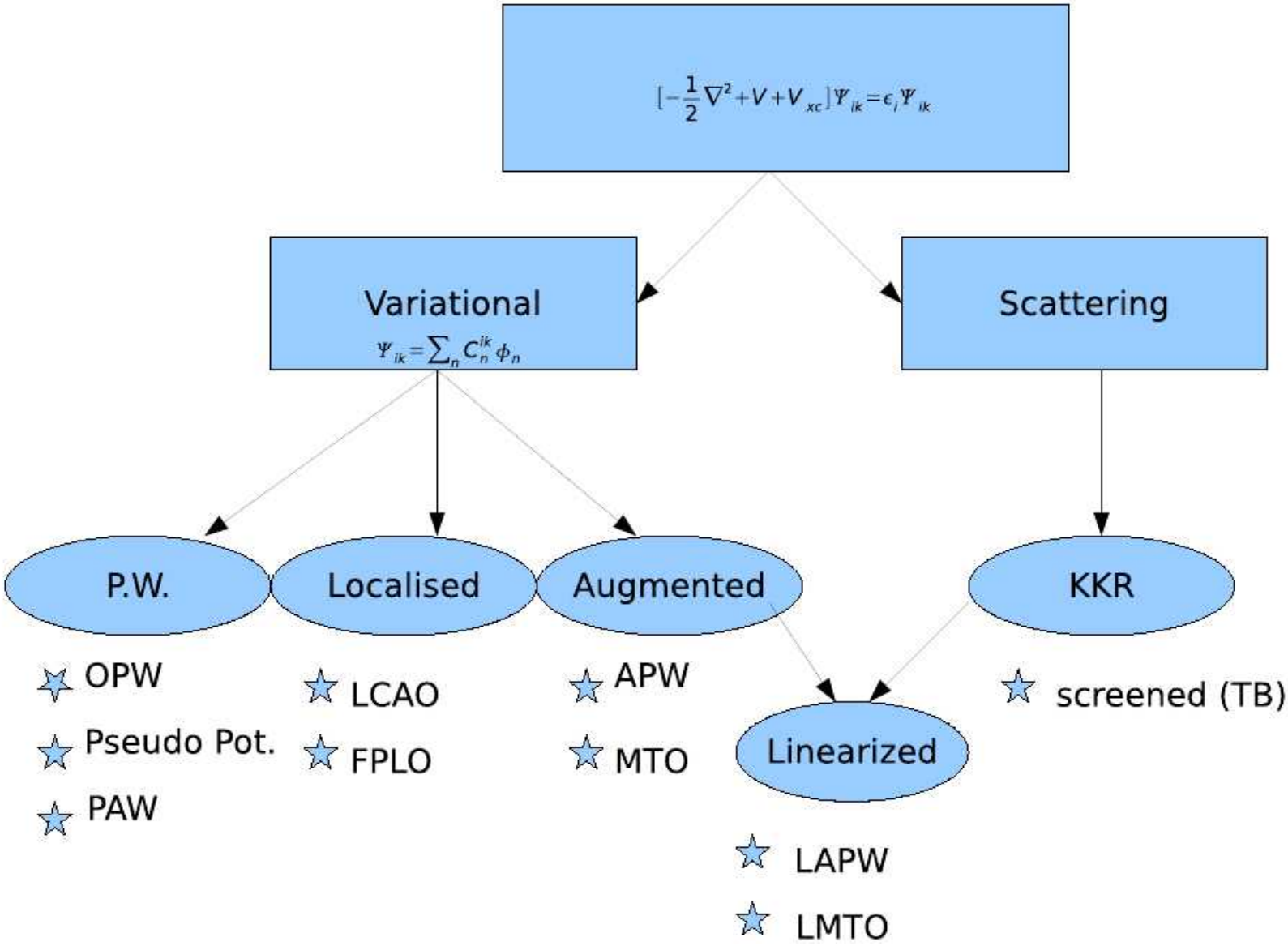
Ansatz: $\Psi_{j\vec{k}}(\vec{r}, E) = \sum_{lm} A_{lm}^{j\vec{k}} R_l(r, E) Y_{lm}(\hat{r})$

Application of variational principle $\Rightarrow$ secular equation

$$\left[\underline{\underline{H}}^{\vec{k}} - E^{j\vec{k}}\underline{\underline{O}}^{\vec{k}}\right]\underline{A}^{j\vec{k}} = \underline{0}$$

$H_{LL'}$	Hamilton matrix
$O_{LL'}$	overlap matrix
$E^{j\vec{k}}$	energy eigenvalue
$A_L^{j\vec{k}}$	eigenvector
$L = (l, m)$	combined angular momentum index

Band structure methods



Original KKR method

Replace differential Schrödinger equation

$$\left[-\vec{\nabla}^2 + V(\vec{r})\right] \psi_{\vec{k}}(\vec{r}, E) = E_{\vec{k}} \psi_{\vec{k}}(\vec{r}, E)$$

by integral Lippmann-Schwinger equation

$$\psi_{\vec{k}}(\vec{r}, E) = e^{i\vec{k}\vec{r}} + \int d^3r'\, G_0(\vec{r}, \vec{r}', E)\, V(\vec{r}')\, \psi_{\vec{k}}(\vec{r}', E)$$

with free electron Green's function $G_0(\vec{r}, \vec{r}', E)$

Korringa, Physica **13** 392 (1947); Kohn, Rostoker, PRB **94** 1111 (1954)

KKR secular equation

Ansatz: $\Psi_{j\vec{k}}(\vec{r}, E) = \sum_{lm} A_{lm}^{j\vec{k}}\, \mathrm{i}^l\, R_l(r, E)\, Y_{lm}(\hat{r})$

Application of variational principle $\Rightarrow$ secular equation

$$\left[\underline{t}(E_{j\vec{k}})^{-1} - \underline{G}_0(\vec{k}, E_{j\vec{k}})\right] A^{j\vec{k}} = 0$$

$\underline{t}(E)$	t-matrix
$\underline{G}_0(\vec{k}, E_{j\vec{k}})$	structure constants matrix

- minimal numerical basis set used ☺
- splitting into potential and geometrical part ☺
- no standard algebraic eigenvalue problem ☹

Green's functions

Spectral representation of Green's function

$\psi_i(\vec{r}, E_i)$ complete and orthogonal set of eigenfuctions

$$\begin{aligned} (E_i - \mathcal{H})\, \psi_i(\vec{r}, E_i) &= 0 \\ (E - \mathcal{H})\, G(\vec{r}, \vec{r}\,', E) &= \delta(\vec{r} - \vec{r}\,') \end{aligned}$$

$G(\vec{r}, \vec{r}\,', E)$ for fixed $\vec{r}\,'$ and E can be expanded into a series of $\psi_i(\vec{r}, E_i)$ (Mercer's theorem)

$$G^+(\vec{r}, \vec{r}\,', E) = \lim_{\epsilon \to 0} \sum_i \frac{\psi_i(\vec{r}) \psi_i^{\times}(\vec{r}\,')}{E - E_i + i\epsilon}$$

retarded Green's function

- poles of $G^+(\vec{r}, \vec{r}\,', E)$ indicate eigenvalues
- $\lim_{\epsilon \to 0}$ avoids divergencies

Densities and expectation values

The Dirac identity $\lim_{\epsilon \to 0} \Im \frac{1}{x + i\epsilon} = -\pi\, \delta(x)$ leads to

$$-\frac{1}{\pi} \Im G^+(\vec{r}, \vec{r}', E) = \sum_i \psi_i(\vec{r}) \psi_i^\dagger(\vec{r}') \delta(E - E_i)$$

$\Im G^+(\vec{r}, \vec{r}', E)$ can be interpreted as density matrix

Density of states $$n(E) = -\frac{1}{\pi} \Im \int_V d^3r\, G^+(\vec{r}, \vec{r}, E)$$

Particle density $$n(\vec{r}) = -\frac{1}{\pi} \Im \int^{E_F} dE\, G^+(\vec{r}, \vec{r}, E)$$

Expectation value $$\langle \mathcal{A} \rangle = -\frac{1}{\pi} \Im \int^{E_F} dE \int_V d^3r\, \mathcal{A}\, G^+(\vec{r}, \vec{r}, E)$$

Analyticity of Green's functions

Extension of $G^+(\vec{r},\vec{r}',E)$ to complex energies z

$$(z-\mathcal{H})\,G(\vec{r},\vec{r}',z) \;=\; \delta(\vec{r}-\vec{r}')$$

with

$$G(\vec{r},\vec{r}',z) \;=\; \sum_i \frac{\psi_i(\vec{r})\psi_i^{\times}(\vec{r}')}{z-E_i}$$

implies $G(\vec{r},\vec{r}',E)$ to be analytical for $\Im z \neq 0$ and

$$G(\vec{r},\vec{r}',z) \;=\; G^{\times}(\vec{r}',\vec{r},z^*)$$

Accordingly one has e.g. for the particle density

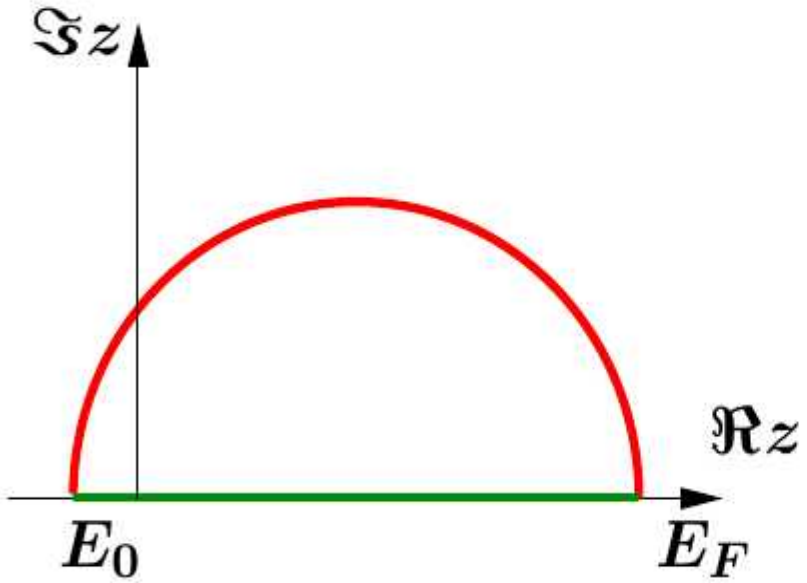
$$n(\vec{r}) = -\frac{1}{\pi}\Im\int_{-}^{E_F} dE\, G^+(\vec{r},\vec{r},E) = -\frac{1}{\pi}\Im\int_{\cap}^{E_F} dz\, G(\vec{r},\vec{r},z)$$

Path integrals in complex energy plane

particle density $n(\vec{r})$

$$n(\vec{r}) = -\frac{1}{\pi}\Im \int_{-}^{E_F} dE\, G^{+}(\vec{r},\vec{r},E)$$

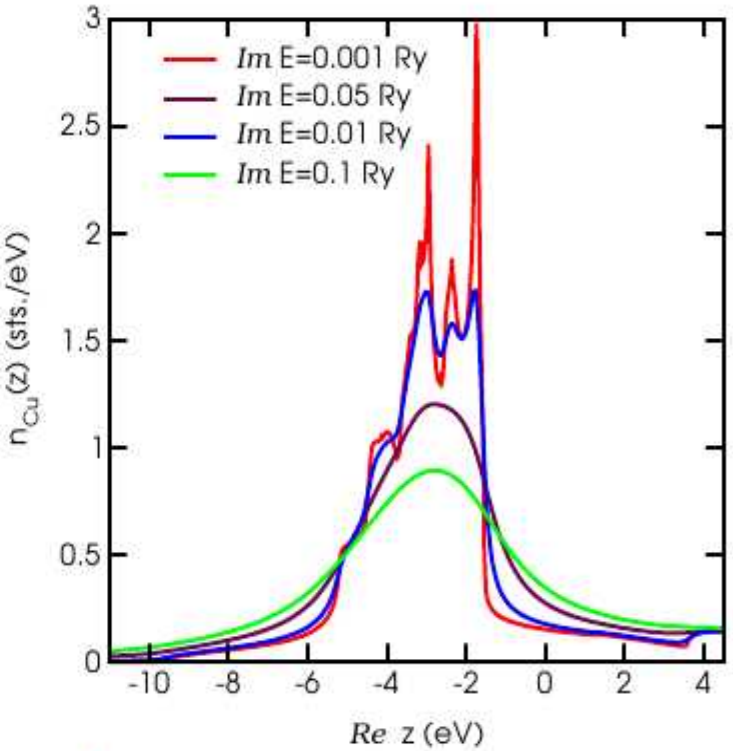
$$= -\frac{1}{\pi}\Im \int_{\cap}^{E_F} dz\, G(\vec{r},\vec{r},z)$$



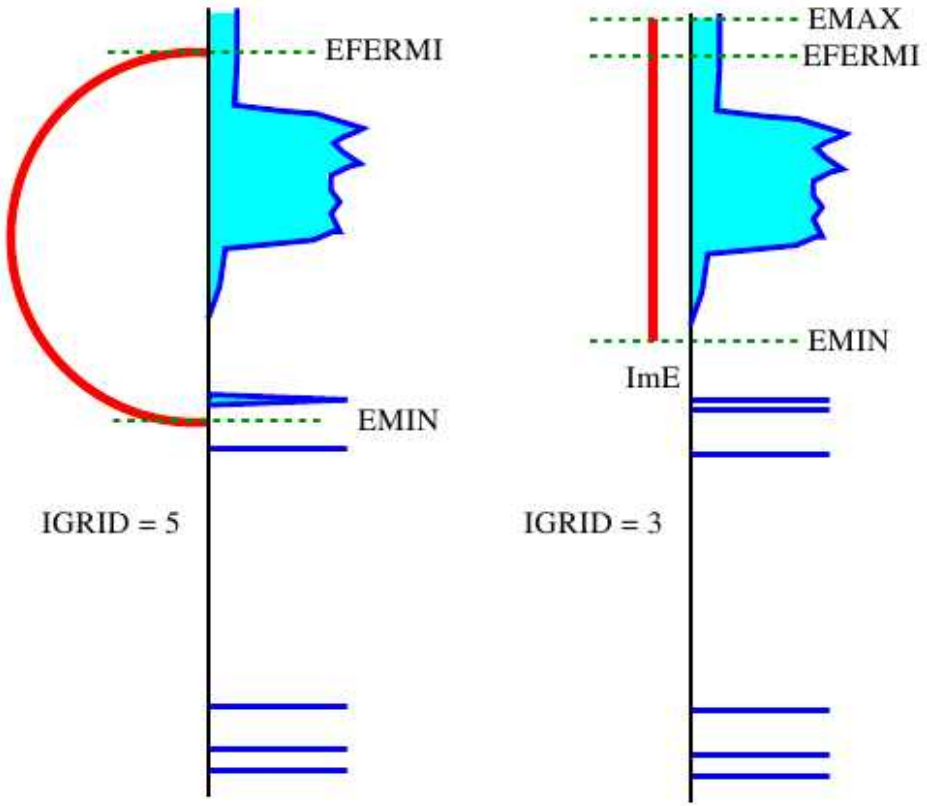
density of states

$$n(z) = -\frac{1}{\pi}\Im \int d^3r\, G(\vec{r},\vec{r},z)$$

for fixed $\Im z$ || real E-axis

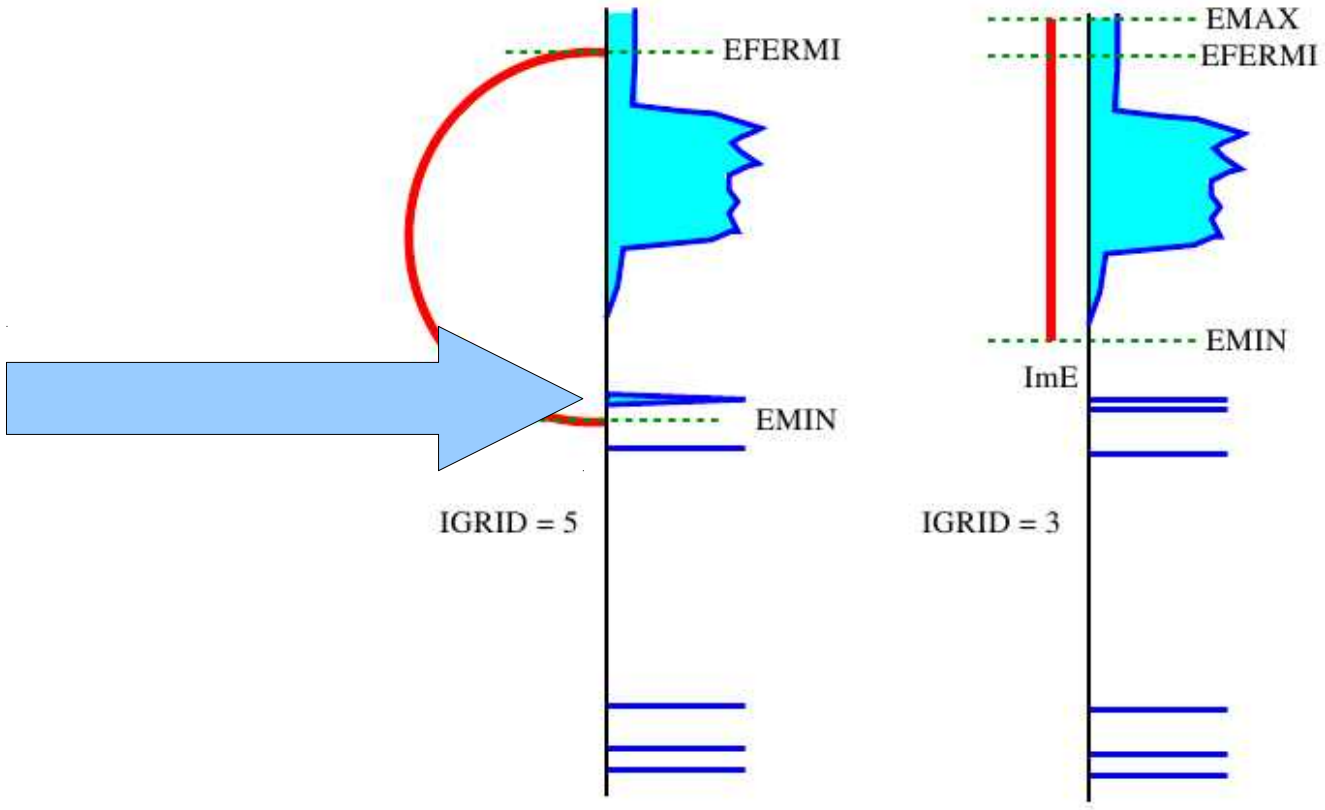


Energy paths



- SCF: arc in the complex plane used for integration
- DOS: straight path along real axis
- XAS: special straight path starting at E_F
- ...

Energy paths



- **Alway take care of semi-core states !**
- SPR-KKR uses automatic search for semi-core states
- Parameter for number of valence electrons: NVAL

Dyson Equation

$\mathcal{H}_0$: Hamiltonian for unperturbed system

$$(E - \mathcal{H}_0) G_0(\vec{r}, \vec{r}', E) = \delta(\vec{r} - \vec{r}')$$

Treatment of perturbed system

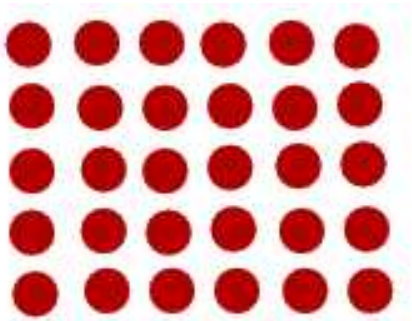
$$\begin{aligned} \mathcal{H} &= \mathcal{H}_0 + V(\vec{r}) \\ (E - \mathcal{H}) G(\vec{r}, \vec{r}', E) &= \delta(\vec{r} - \vec{r}') \end{aligned}$$

solution supplied by Dyson equation

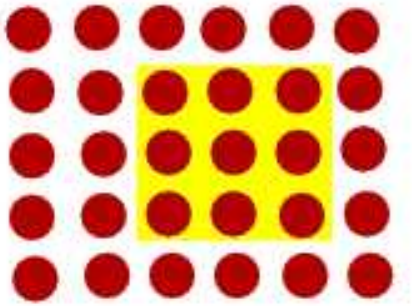
$$\begin{aligned} G(\vec{r}, \vec{r}', E) &= G_0(\vec{r}, \vec{r}', E) \\ &\quad + \int d^3 r'' \, G_0(\vec{r}, \vec{r}'', E) \, V(\vec{r}'') \, G(\vec{r}'', \vec{r}', E) \end{aligned}$$

Example: Dyson equation applied to 0D systems

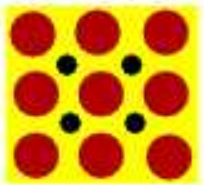
I **SCF calculations for unperturbed host**



II **Calculation of G^0 for selected host region Ω**



III **Application of Dyson equation**
$G = G^0 + G\Delta V G^0$
for embedded system



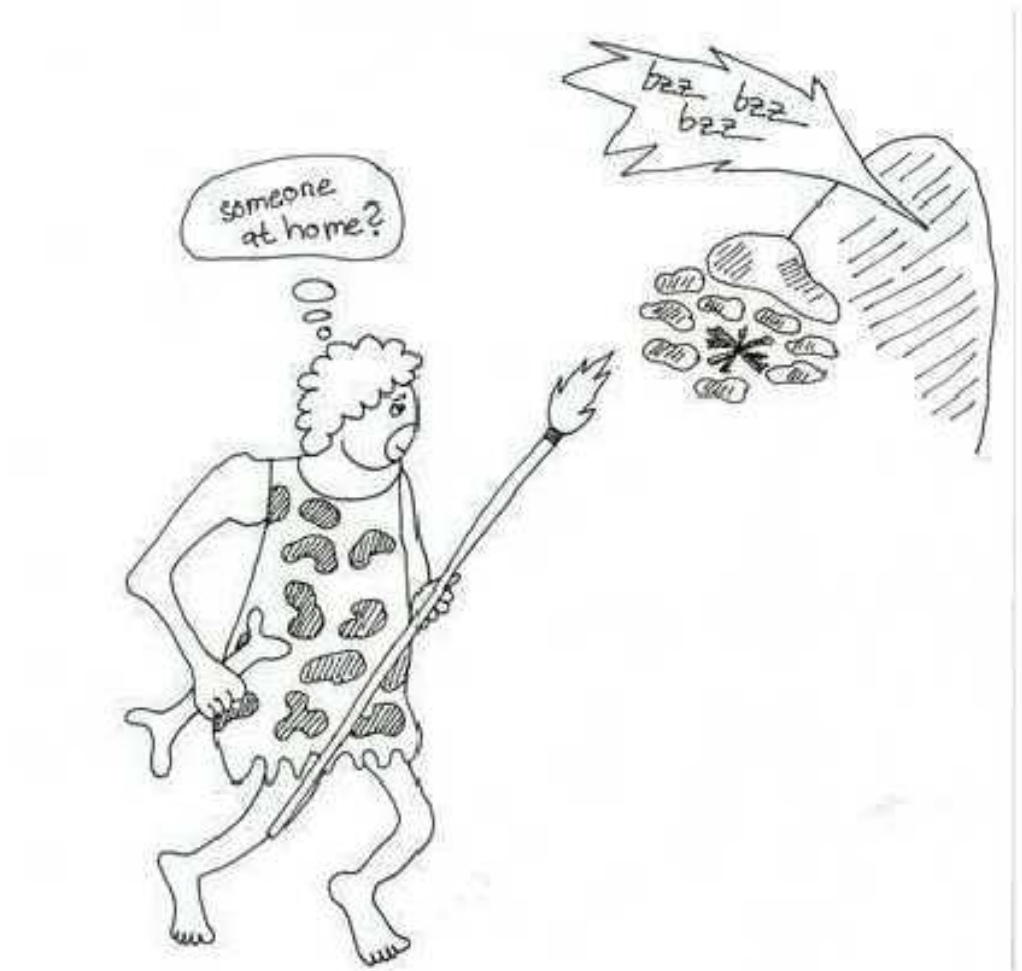
Benefits of Green's function based methods

Straightforward application to

- any type of host/impurity system
- surfaces or arbitrary layered systems
- disordered systems using appropriate alloy theory
- response to an external perturbation
  - susceptibilities
  - transport properties
  - spectroscopy
- many-body problems
- etc.

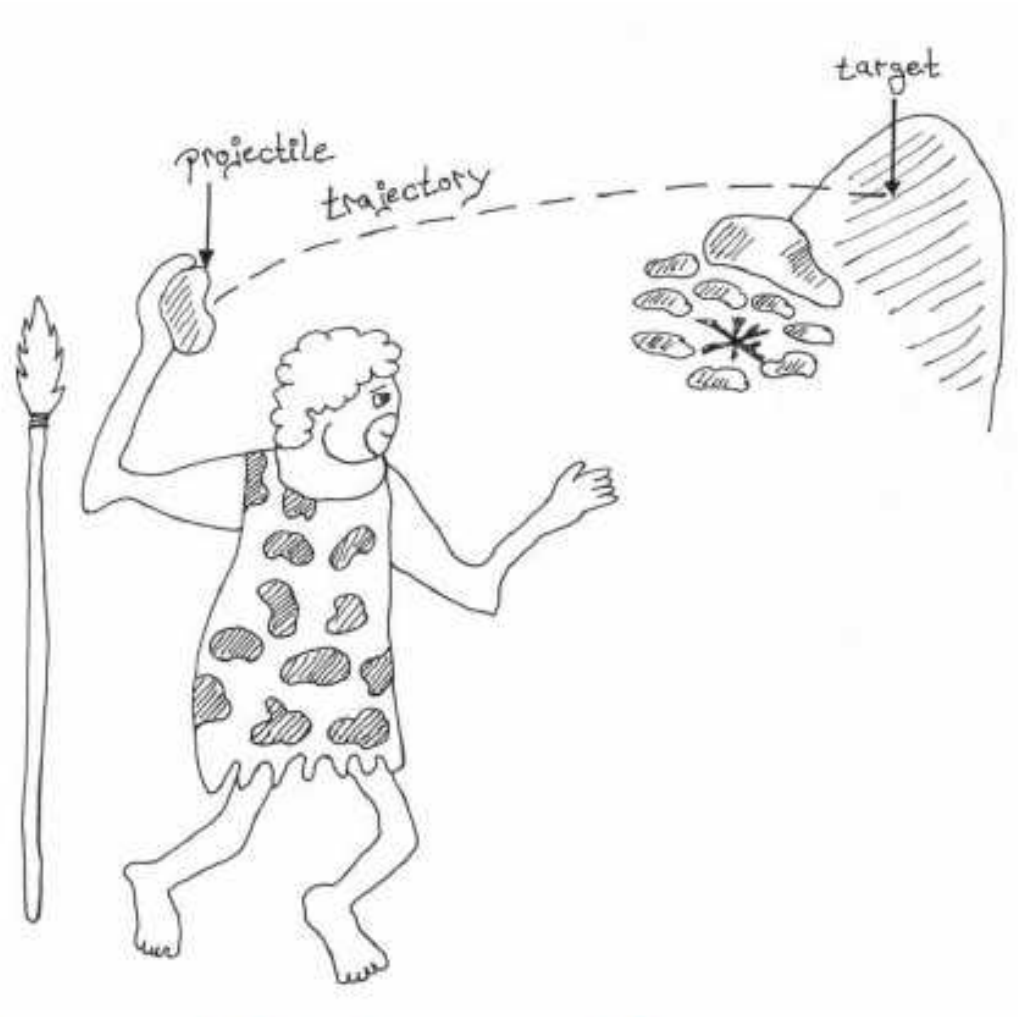
It's worth to work with Green's functions ...
... but how to calculate them ???

Early applications of scattering theory



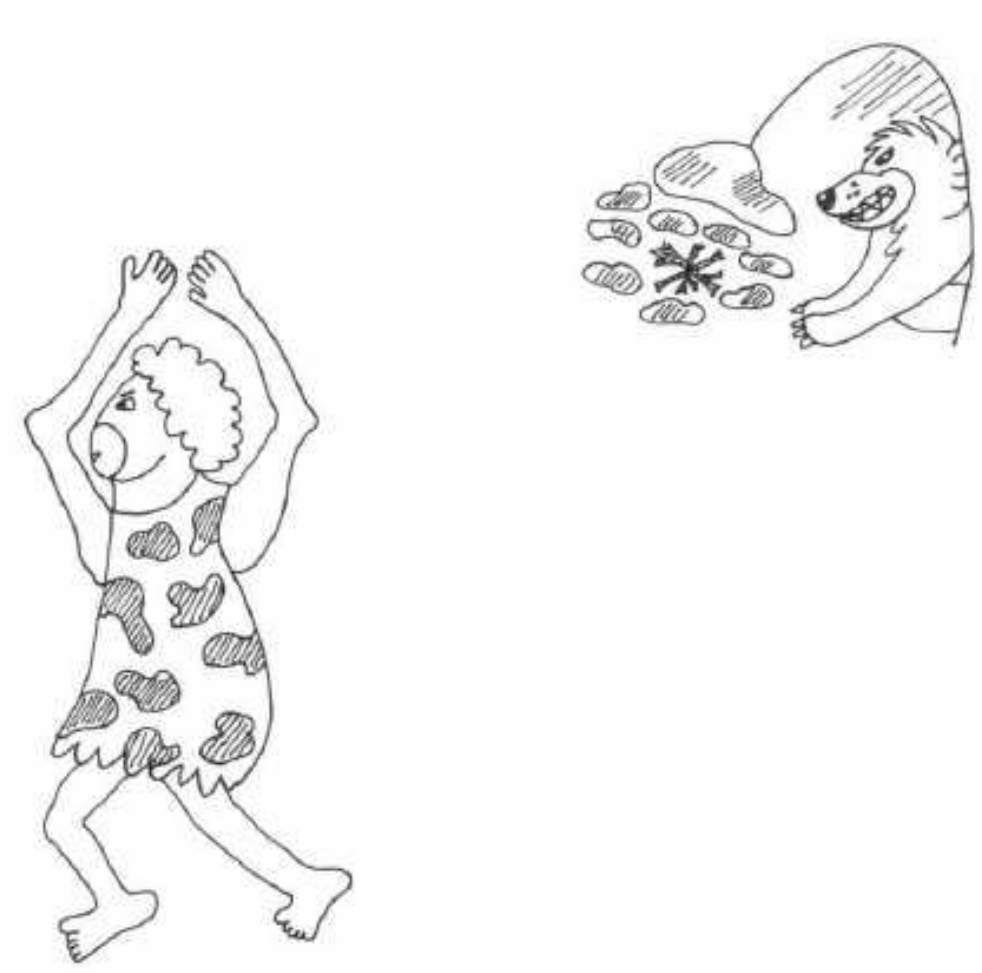
... for solving problems

Principle of scattering theory



... to get information on a target

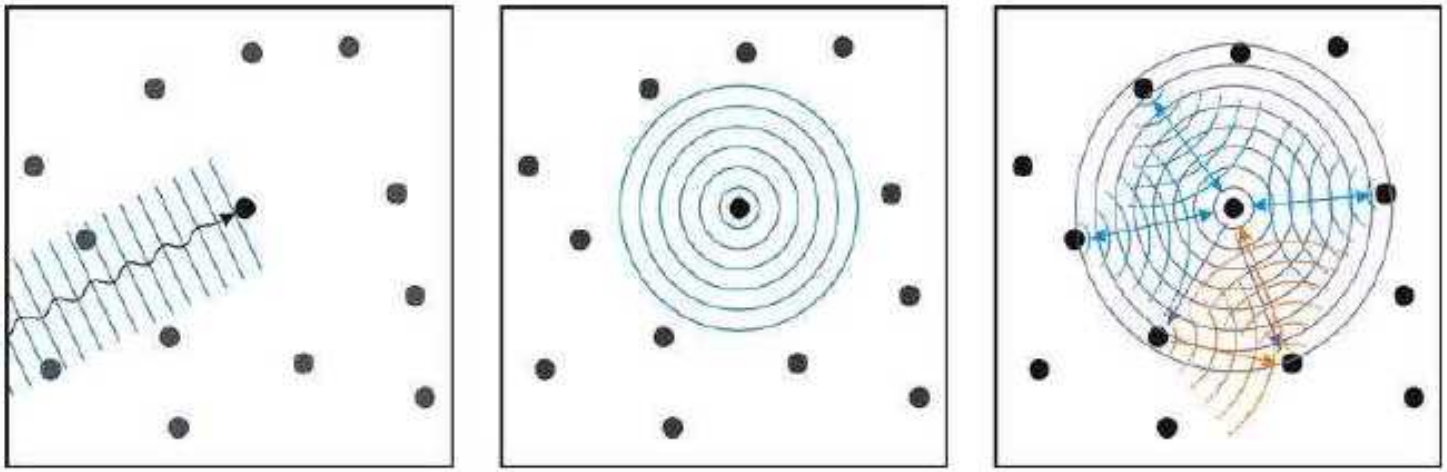
Sometimes solving a problem ....



... leads to another one

Calculation of the Green's function

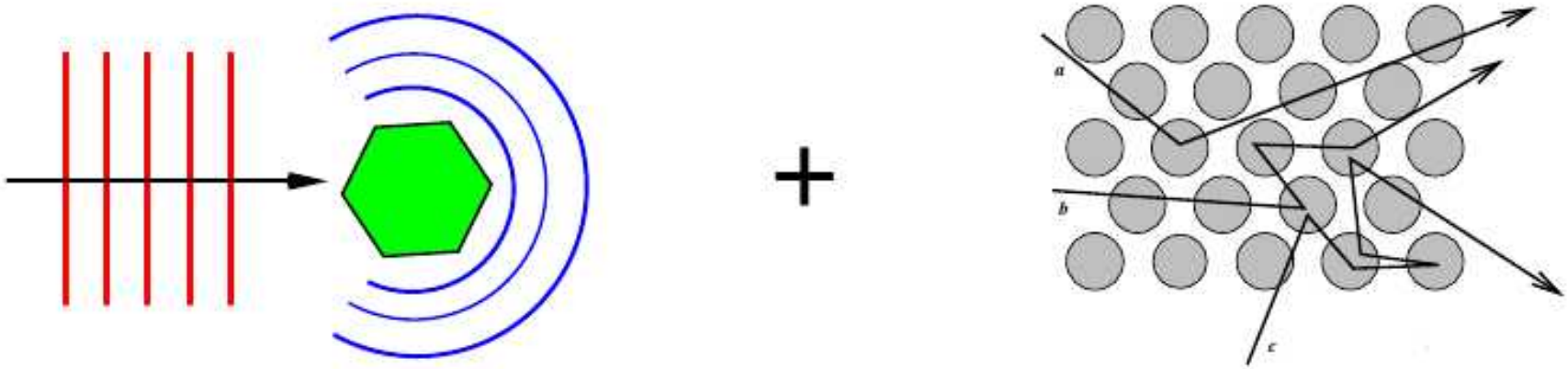
Use the concept of EXAFS theory



for electronic structure calculations

$\Rightarrow$ KKR $\equiv$ multiple scattering theory

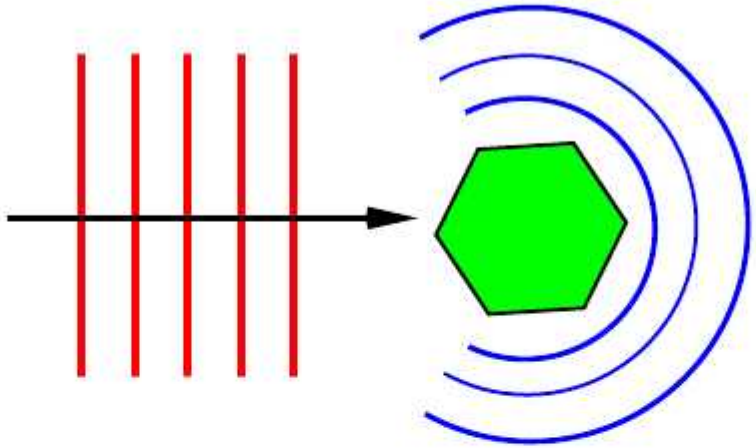
Calculation of the Green's function: KKR



- separate structural information and information of scatterers
- G determined by self-consistent multiple scattering formalism

Single site scattering problem

Standard problem in a scattering experiment
scattering of a plane wave at a target



Lippmann-Schwinger equation

$$\psi(\vec{r}, E) = e^{i\vec{k}\vec{r}} + \int_{\Omega_n} d^3r'\, G_0(\vec{r}, \vec{r}', E)\, V^n(\vec{r})\, \psi(\vec{r}, E)$$

$$= e^{i\vec{k}\vec{r}} + \int_{\Omega_n} d^3r' \int_{\Omega_n} d^3r''\, G_0(\vec{r}, \vec{r}', E)\, t^n(\vec{r}', \vec{r}'', E)\, e^{i\vec{k}\vec{r}''}$$

with $|\vec{k}| = \sqrt{E}$

Angular momentum expansion of $\psi(\vec{r}, E)$

Solving the Schrödinger equation

$$\left[-\vec{\nabla}^2 + V(r)\right] \psi(\vec{r}, E) = E\psi(\vec{r}, E)$$

using the ansatz

$$\psi(\vec{r}, E) = \sum_L R_l(r, E) Y_L(\hat{r})$$

leads to the radial Schrödinger equation

$$\left[-\frac{\partial^2}{\partial r^2} + \frac{l(l+1)}{r^2} + V(r)\right] R_l(r, E) = 0$$

for the radial wave function $R_l(r, E)$

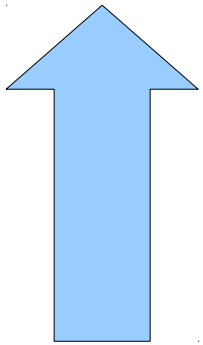
Angular momentum expansion of $\psi(\vec{r}, E)$

Solving the Schrödinger equation

$$\left[-\vec{\nabla}^2 + V(r)\right] \psi(\vec{r}, E) = E\psi(\vec{r}, E)$$

using the ansatz

$$\psi(\vec{r}, E) = \sum_L R_l(r, E) Y_L(\hat{r})$$



NLMAX=l_max+1: is in KKR convergence criteria

Often helps to use Lloyd formula: LLOYD option
(for insulators and semiconductors)

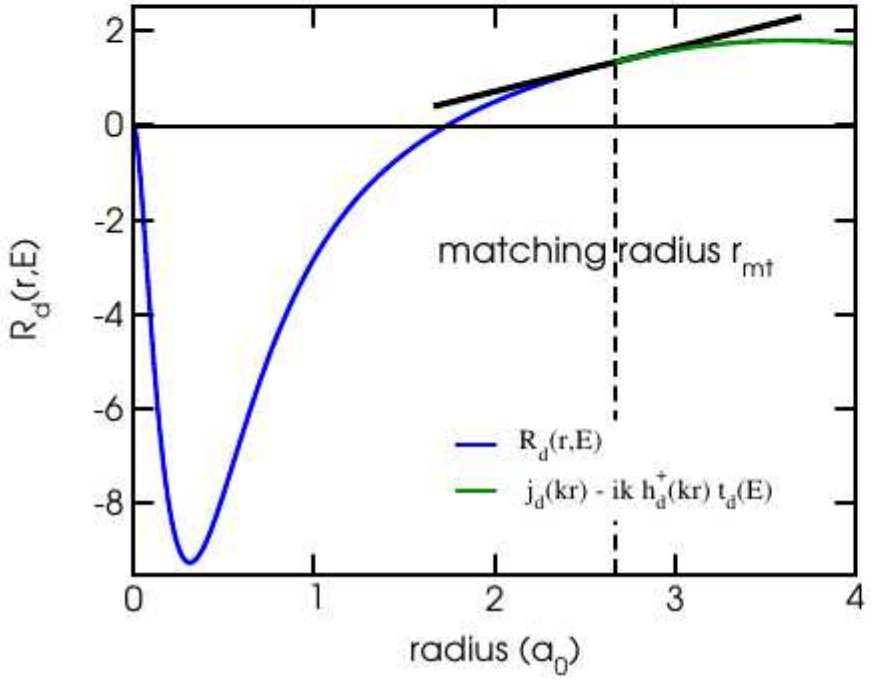
Expression for the single site *t*-matrix

Matching at the muffin-tin radius

$$\tilde{R}_l(r,E)\cdot N_l(E) = R_l(r,E) \;\rightarrow\; j_l(kr) - ikh_l^+(kr)t_l(E)$$

$$\frac{d}{dr}R_l(r,E) \;\rightarrow\; \frac{d}{dr}\left[j_l(kr) - ikh_l^+(kr)t_l(E)\right]$$

$\tilde{R}_l$: unnormalised solution of radial Schrödinger equation



$$t_l(E) = -\frac{1}{ik}\frac{\left[j_l,\tilde{R}_l\right]_{r=r_{\mathrm{mt}}}}{\left[h_l^+,\tilde{R}_l\right]_{r=r_{\mathrm{mt}}}}$$

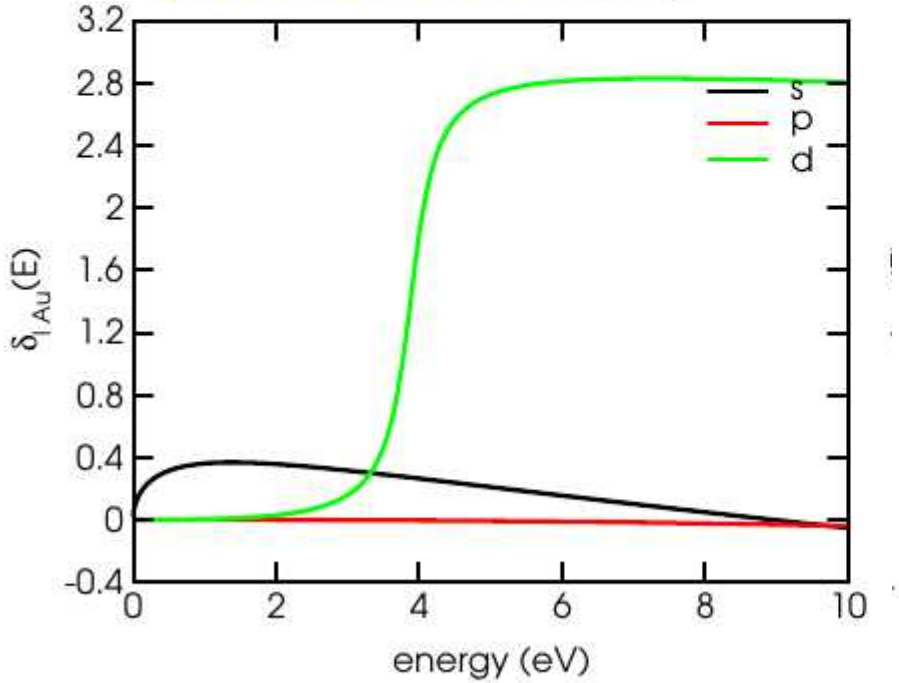
Wronskian

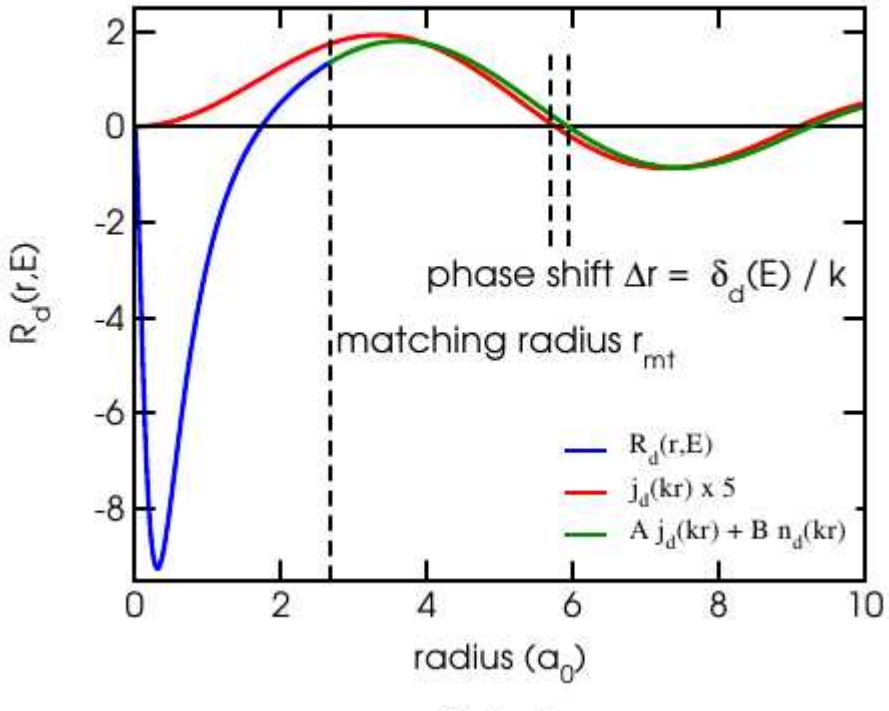
$$[u,v] = u(r)\frac{d}{dr}v(r) - v(r)\frac{d}{dr}u(r)$$

Phase shift $\delta_l(E)$ and single site t-matrix

$$t_l(E) = -\frac{1}{k}\,\sin\left(\delta_l(E)\right)\,e^{i\delta_l(E)}$$

phase shift $\delta_l(E)$





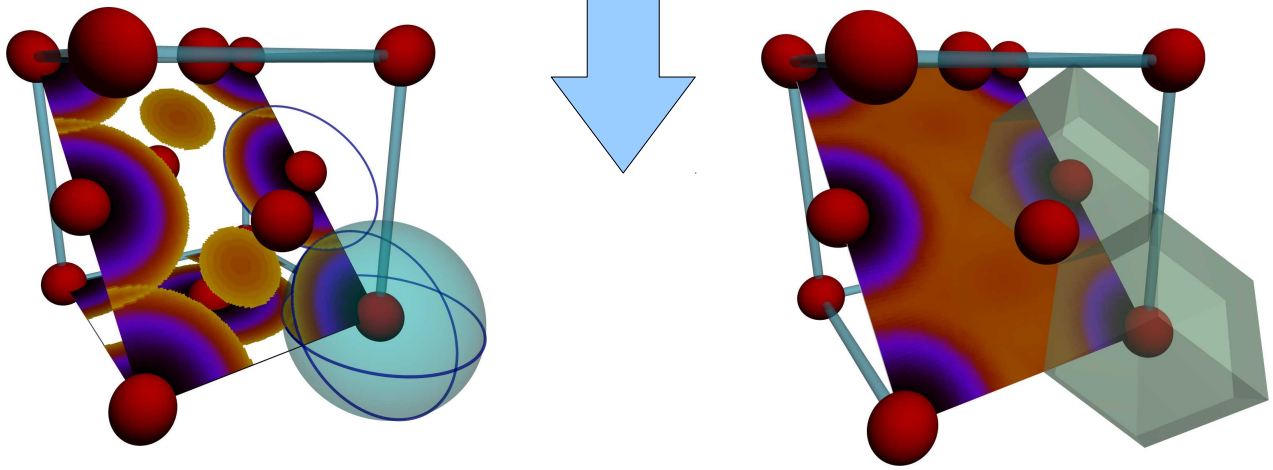
scalar-relativistic results for Au

Single site problem in SPR-KKR

Default in SPR-KKR: The Dirac Equation within SDFT

$$\left[\frac{\hbar}{i}c\vec{\alpha}\cdot\vec{\nabla}+\beta mc^2+\bar{V}(\vec{r})+\underbrace{\beta\vec{\sigma}\cdot\vec{B}_{\rm eff}(\vec{r})}_{V_{\rm spin}(\vec{r})}\right]\Psi(\vec{r},E)=E\,\Psi(\vec{r},E)$$

ASA **Full-potential**



- ASA: keep the volume of the unit cell constant
  - assume a spherical symmetric potential within sphere
- FP: Space filling Wigne-Seitz cell
  - Total energies tested and compared with LAPW
  - NEW: FP implementation in fully relativistic mode (Left + Right hand side solution to Dirac eq.
  - Not all applications are implemented in FP mode yet

Single site problem in SPR-KKR

Default in SPR-KKR: The Dirac Equation within SDFT

$$\left[\frac{\hbar}{i}c\vec{\alpha}\cdot\vec{\nabla}+\beta mc^2+\bar{V}(\vec{r})+\underbrace{\beta\vec{\sigma}\cdot\vec{B}_{\mathrm{eff}}(\vec{r})}_{V_{\mathrm{spin}}(\vec{r})}\right]\Psi(\vec{r},E)=E\,\Psi(\vec{r},E)$$

- Fully relativistic mode (4-component formalism)
- Scalar relativistic
- Non-relativistic
- Spin spiral calculations

- LSDA, GGA
- Rotational invariant LSDA+U
- Fully self consitent (charge + self energy) LSDA+DMFT
- Breit interaction
- SOC manipulations

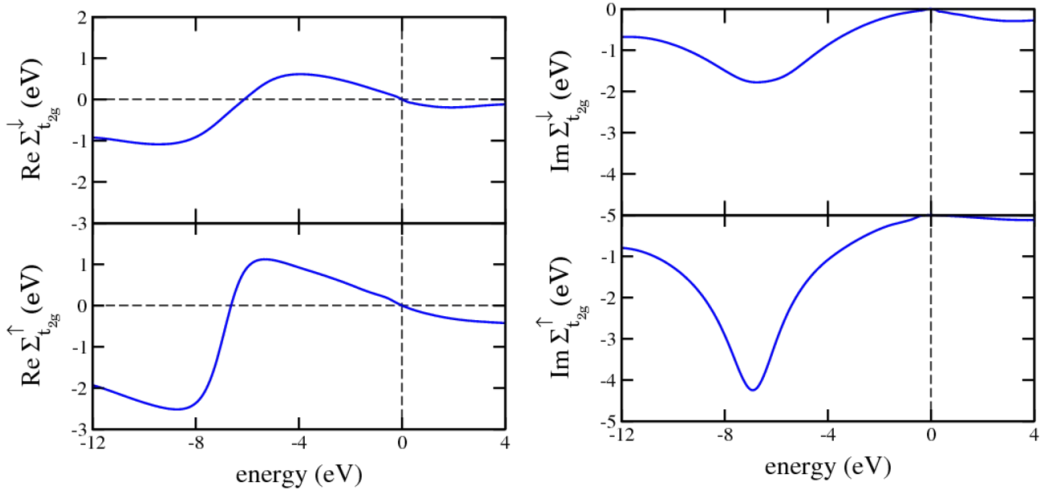
Implementation of LSDA+DMFT using KKR

Dyson equation:

$$G(\vec{r},\vec{r}\,',E) = G_0(\vec{r},\vec{r}\,',E) + \int \mathrm{d}^3r'' \int \mathrm{d}^3r''' G_0(\vec{r},\vec{r}\,'',E) \left[V_{\mathrm{LSDA}}(\vec{r}\,'')\delta(\vec{r}\,''-\vec{r}\,''') + \Sigma(\vec{r}\,'',\vec{r}\,''',E)\right] G(\vec{r}\,''',\vec{r}\,',E)$$

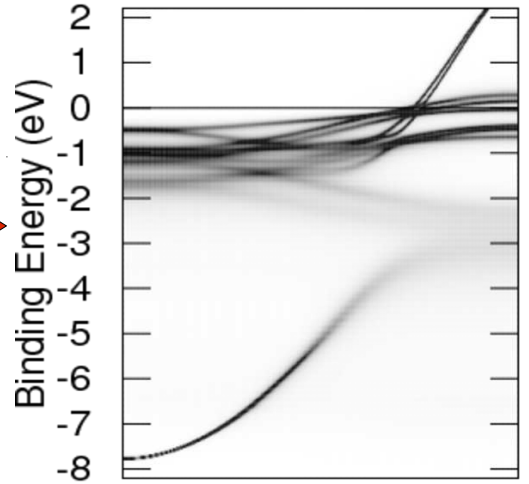
with $\Sigma(\vec{r},\vec{r}\,',E)$ *on-site* self-energy.

Spin dependent self energy of Ni for d-states

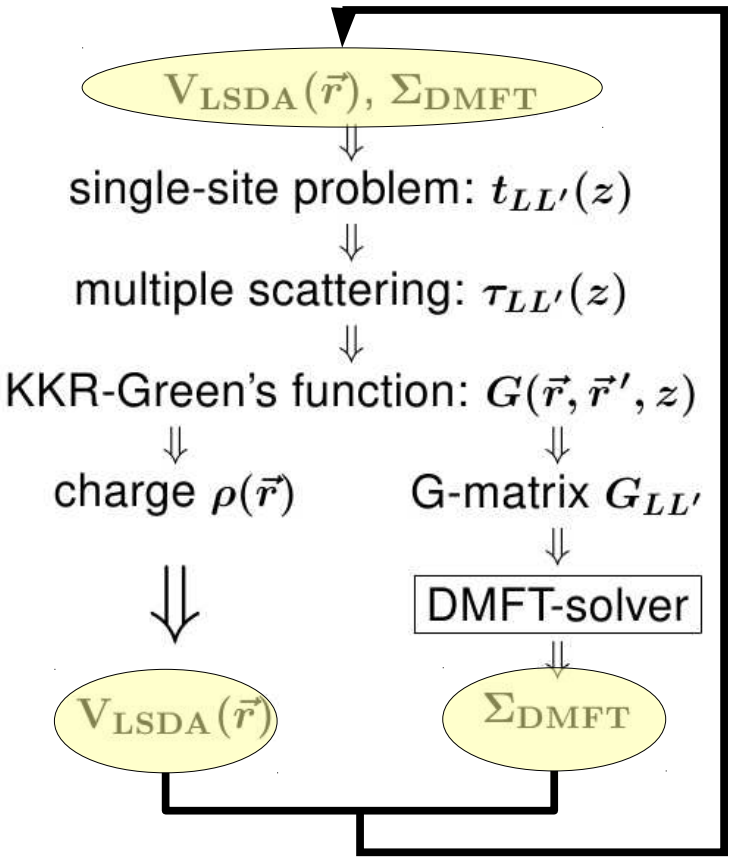


Real part Imaginary part

Bloch spectral function



Implementation of LSDA+DMFT using KKR



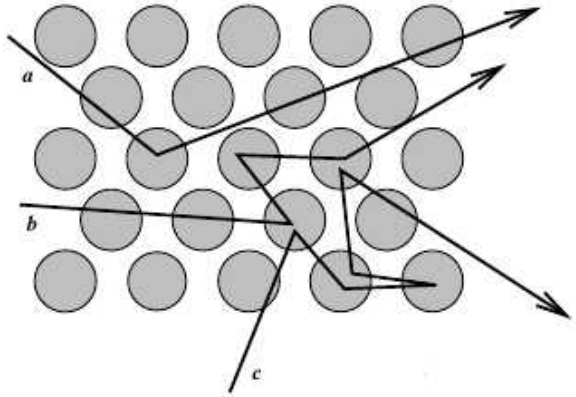
$$\left[\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}r - \frac{l(l+1)}{r^2} - V^{\sigma}(r) + E\right]\psi_L(r,E)$$

$$= \sum_{L''}\int r'^2 \mathrm{d}r'\, \Sigma^{\sigma}_{LL''}(E)\,\phi_l(r)\,\phi_{l''}(r')\,\psi_L(r',E)$$

- Fully self-consistent (charge + Σ_{DMFT})
- Fully relativistic (Dirac eq.)
- Σ_{DMFT} solver: SPTF (I. Di Marco el al.) and TMA (Chadov et al.)
- Effects of Σ_{DMFT} on wave functions
- Disordered alloys: CPA+DMFT and 2D semi-infinite surfaces
- Spectroscopies + DMFT: ARPES, XAS, XMCD,MOKE …

J. Minar, et al, PRB **72**, 045125 (2005),
JPCM Topical review 23, 253201 (2011)
Applications see e.g.: PRL **95,** 166401 (2005), **97**, 227601 (2006), PRL 103, 267203 (2009),

Multiple scattering



scattering T-matrix operator of the crystal $\hat{T}$

$$\hat{T} = \sum_{n} \hat{t}^{n} + \sum_{n,m} \hat{t}^{n}\,\hat{G}_0\,\hat{t}^{m} + \sum_{\substack{n,m,k \\ n,m\neq k}} \hat{t}^{n}\,\hat{G}_0\,\hat{t}^{m}\,\hat{G}_0\,\hat{t}^{k} + \cdots$$

decomposition into scattering path operator $\hat{\tau}^{nm}$

$$\hat{T} = \sum_{n,m} \hat{\tau}^{nm}$$

Scattering part operator $\hat{\tau}^{nm}$

self-consistent requirement for $\hat{\tau}^{nm}$
in angular momentum representation

$$\tau^{nm}_{\Lambda\Lambda'} = t^{n}_{\Lambda\Lambda'}\delta_{nm} + \sum_{\Lambda''\Lambda'''} t^{n}_{\Lambda\Lambda''} \sum_{k\neq n} G^{0\,nk}_{\Lambda''\Lambda'''}\tau^{km}_{\Lambda'''\Lambda'}$$

$$\underline{\tau}^{nm} = \underline{t}^{n}\delta_{nm} + \underline{t}^{n} \sum_{k\neq n} \underline{G}^{0\,nk}\underline{\tau}^{km}$$

formal solution

$$\underline{\underline{\tau}} = [\underline{\underline{t}}^{-1} - \underline{\underline{G}}]^{-1}$$

Electronic Green's function

Combining $\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \sum_{n,m} \tau^{nm} \mathcal{G}_0$

$$
\begin{aligned}
G^{ss}(\vec{r},\vec{r}',E) &= \langle \vec{r} | \mathcal{G}_0 + \mathcal{G}_0\, t\, \mathcal{G}_0 | \vec{r}' \rangle \\
&= \sum_L Z_L(\vec{r},E) t_l(E) Z^{\times}_{L'}(\vec{r}',E) \\
&\quad - \sum_L Z_L(\vec{r},E) J^{\times}_L(\vec{r}',E)
\end{aligned}
$$

$$
G_0(\vec{r}_n,\vec{r}_m{}',E) = \sum_{LL'} j_L(\vec{r}_n,E) G^{nm}_{0\,LL'}(E) j^{\times}_{L'}(\vec{r}_m{}',E) \quad (n \neq m)
$$

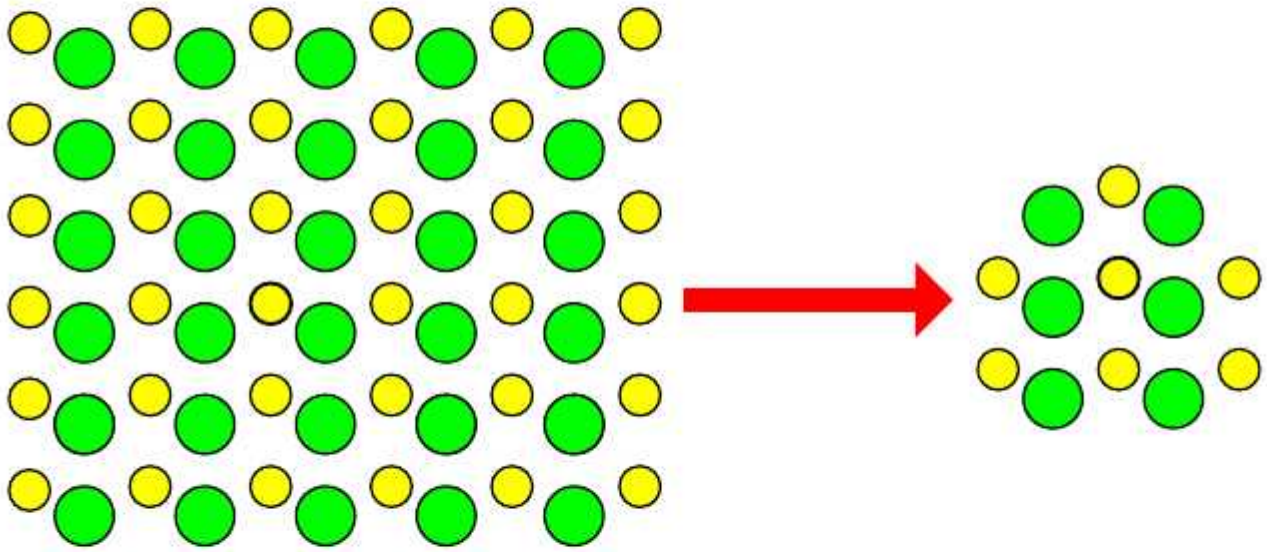
leads to

$$
\begin{aligned}
G(\vec{r}_n,\vec{r}_m{}',E) &= \sum_{LL'} Z_L(\vec{r}_n,E)\, \tau^{nm}_{LL'}(E)\, Z^{\times}_{L'}(\vec{r}_m{}',E) \\
&\quad - \delta_{nm} \sum_L Z_L(\vec{r}_n,E)\, J^{\times}_L(\vec{r}_n{}',E)
\end{aligned}
$$

Solving the multiple scattering problem: Real space

- cluster approximation

cut a finite cluster out of the infinite system centred on the atom of interest



applied e.g. for EXAFS calculations

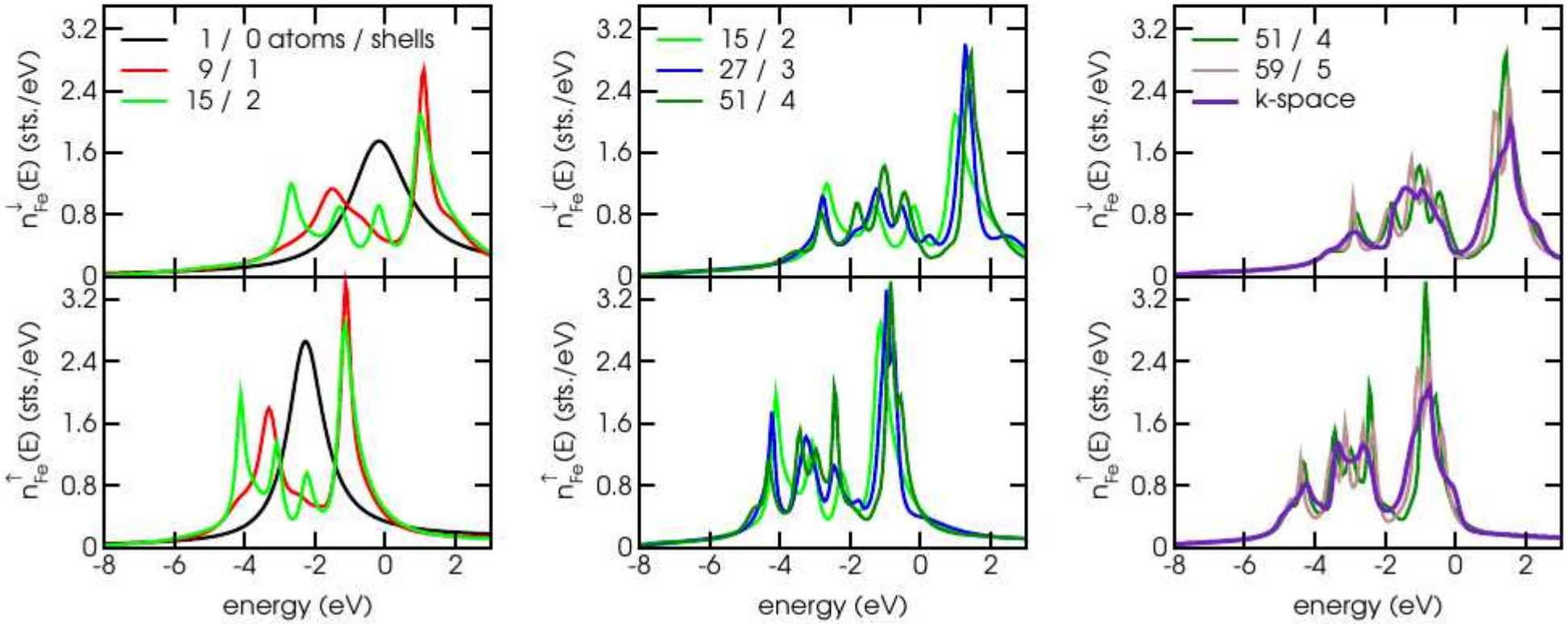
- free clusters and molecules

Solving the multiple scattering problem: Real space

Convergence of cluster approximation

$\underline{\underline{\tau}}(E) = \left[\underline{\underline{t}}(E)^{-1} - \underline{\underline{G}}_0(E) \right]^{-1}$ with cluster size

DOS for central atom of bcc-Fe clusters

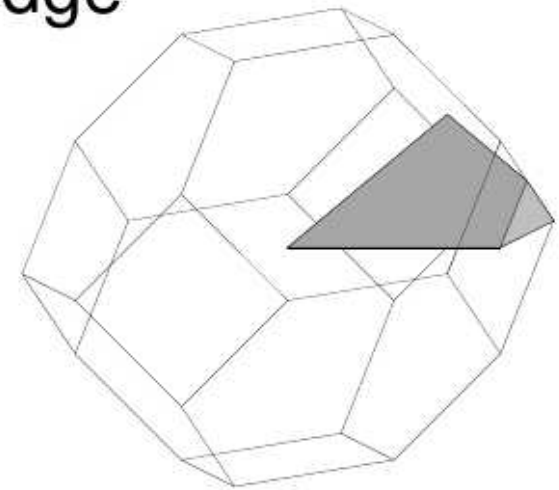


Brillouin zone integration

$$\tau^{nn'}_{\Lambda\Lambda'}(E) = \frac{1}{\Omega_{\mathrm{BZ}}} \int_{\Omega_{\mathrm{BZ}}} d^3k \; e^{i\vec{k}(\vec{R}_n - \vec{R}_{n'})}$$

$$\times [\underbrace{\underline{t}^{-1}(E) - \underline{G}(\vec{k}, E)}_{\text{KKR matrix } M(\vec{k},E)}]^{-1}_{\Lambda\Lambda'}$$

Symmetry allows to reduce the integration regime $\hat{\Omega}_{\mathrm{BZ}}$ to an irreducible wedge



Brillouin zone integration

$$\tau^{nn'}_{\Lambda\Lambda'}(E) = \frac{1}{\Omega_{\mathrm{BZ}}} \int_{\Omega_{\mathrm{BZ}}} d^3k \; e^{i\vec{k}(\vec{R}_n - \vec{R}_{n'})}$$

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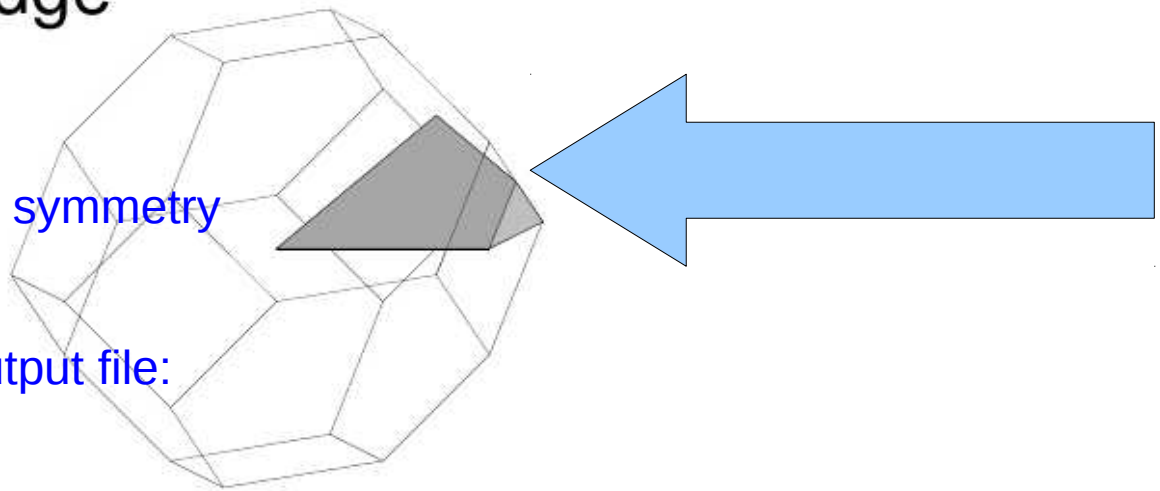
Symmetry allows to reduce the integration regime $\hat{\Omega}_{\mathrm{BZ}}$ to an irreducible wedge

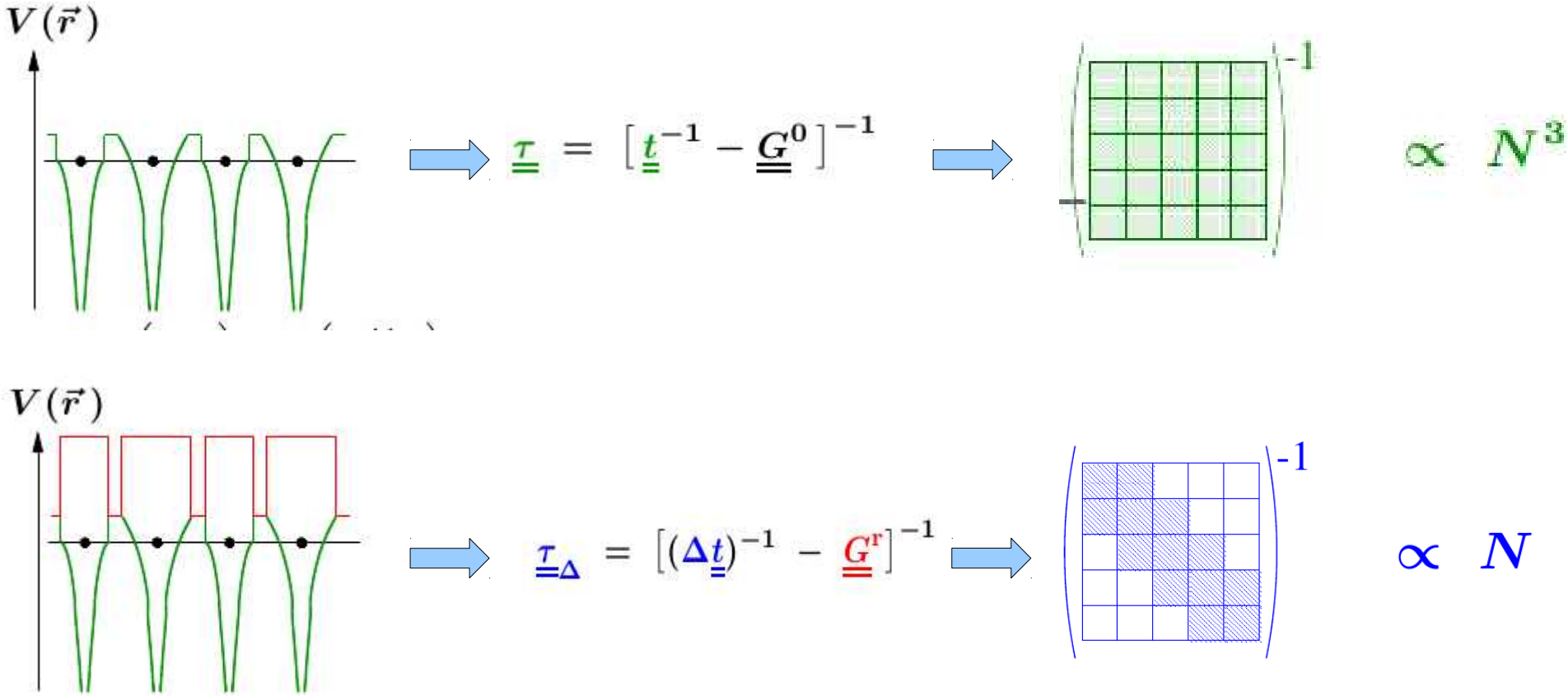


- Special points method: e.g. Use of symmetry
- Input Number of k-points:

NKTAB gives “density” of k-points

- For actual calculations look into output file:
  - mesh parameters

Tight binding or screened KKR method

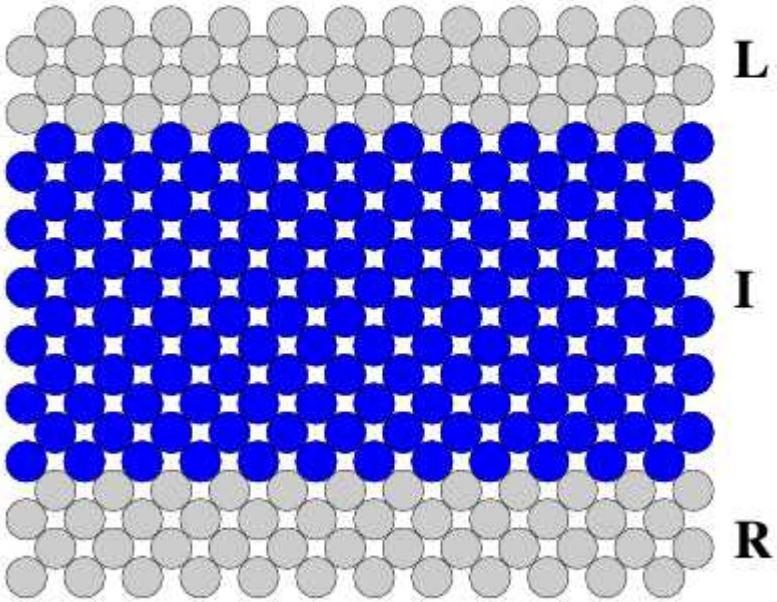


- Standard KKR structure constants are long-ranged (disadvantage)
- Screened KKR structure constants are obtained from a reference medium consisting of repulsive potentials (damped propagation, sparse matrices)

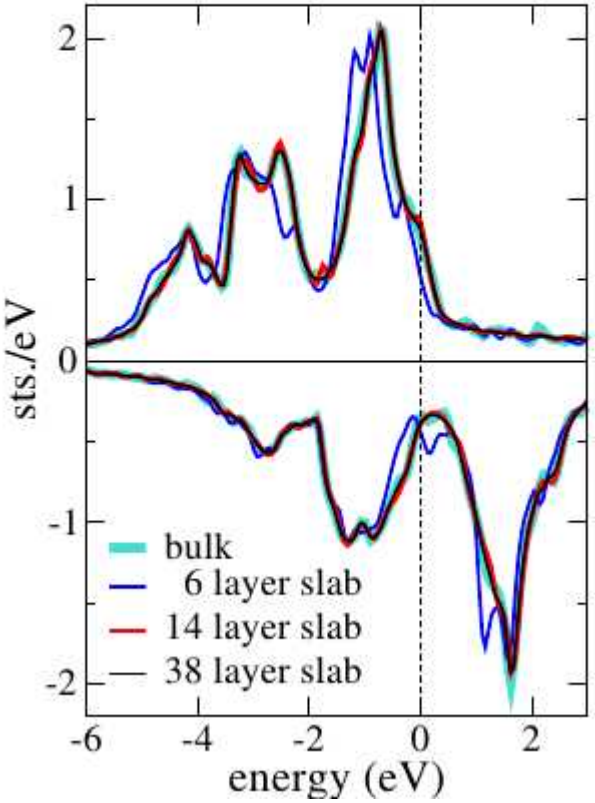
R. Zeller et al.
PRB **49**, 2721 (1994)
PRB **52**, 8807 (1995)

Surface calculations: Slab geometry

finite system

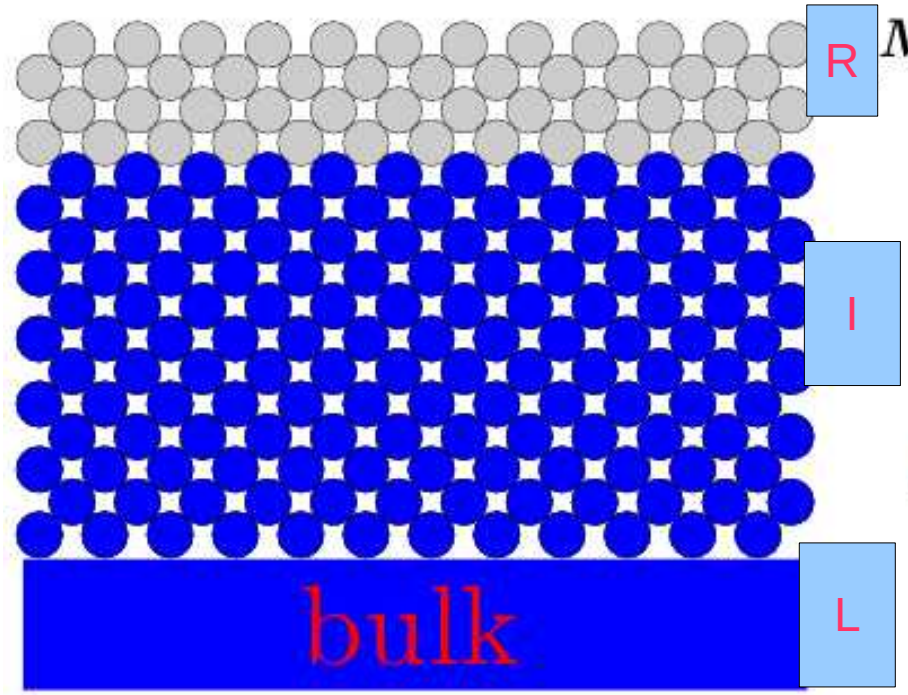


DOS of central slab layer for Fe(001) surface



Surface calculations: semi infinite 2D systems

semi-infinite system



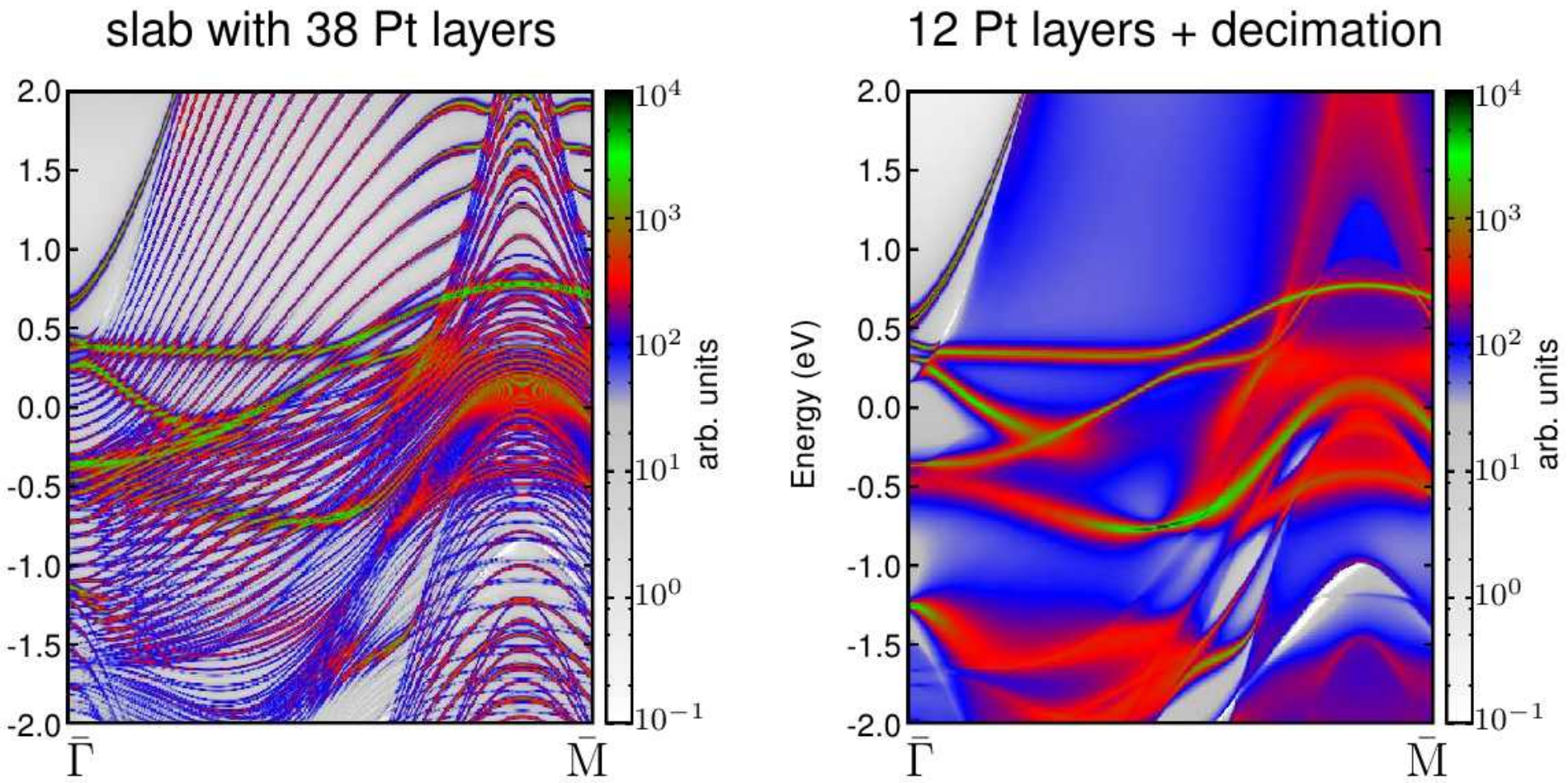
KKR matrix

$$M = \begin{pmatrix} M_{LL} & M_{LI} & 0 \\ M_{IL} & M_{II} & M_{LR} \\ 0 & M_{RI} & M_{RR} \end{pmatrix}$$

- calculation of M_{RR} via decimation or "layer doubling"

Comparison between slab and semi-infinite systems

Projected band structure of a Co monolayer on Pt(111)



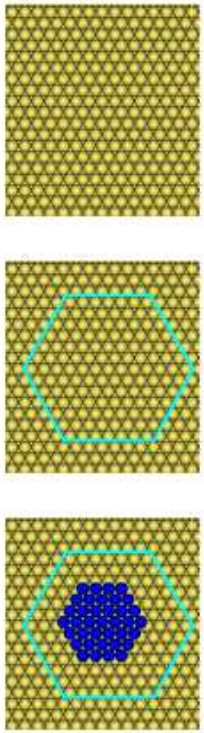
Problems: For 2D systems take care of slow convergence
(use smaller SCFMIX and MIXRHO

O. Sipr et al. PRB 82, 174414 (2010)

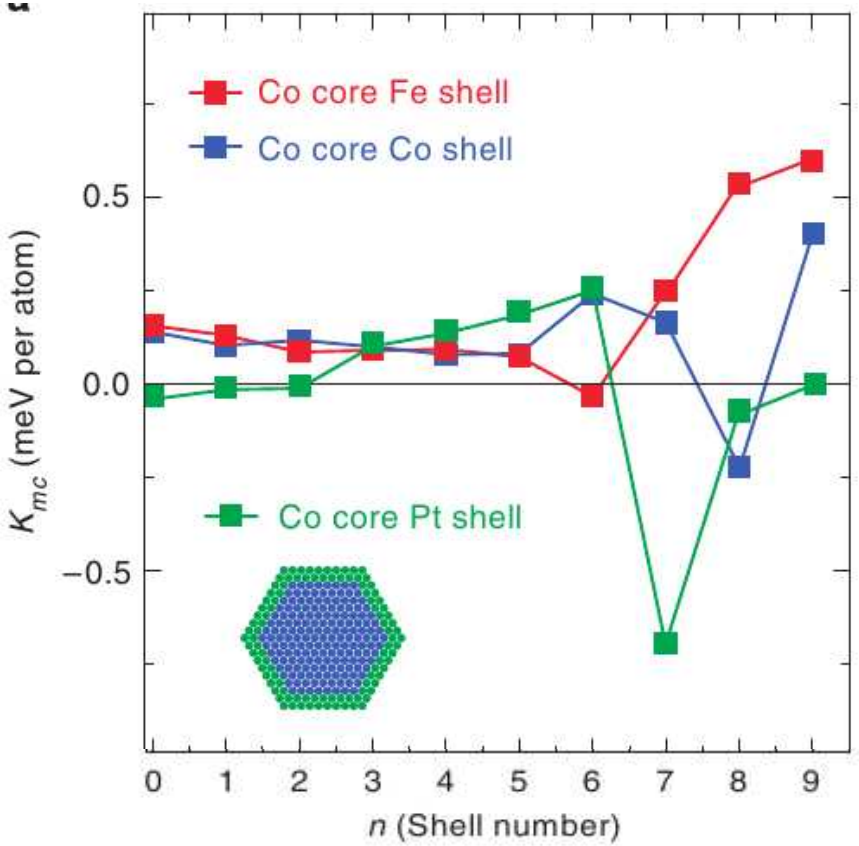
Clusters on Surfaces example

1. SCF calculation for uncovered substrate e.g. Pt(111) surface
2. Calculation of G^0_{ij} for finite substrate region
3. Application of Dyson equation for surface deposited clusters

$$G = G^0 + G\Delta V G^0$$



Shell resolved magneto-crystalline anisotropy

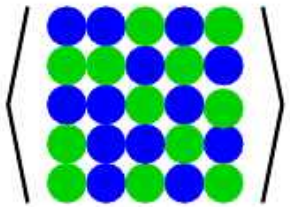


S. Ouazi et al., Nat. Comm. 3, 1313 (2012)

- Embedding in 3D-bulk very well tested and works in ASA and FP
- Embedding on 2D-surface: in ASA OK but in FP still to be tested

Substitional disordered alloys

Electronic structure of a disorderd alloy A_xB_{1-x}
represented by configurational average
for given concentration and eventually short range order



- Super cell technique
- Single site approximation: ignore short range order
  - VCA: Virtual Crystal Approximation
  - ATA: Average t-matrix Approximation
  - CPA: Coherent Potential Approximation
- Cluster approximation: allow short range order
  - NL-CPA: non-local Coherent Potential Approx.

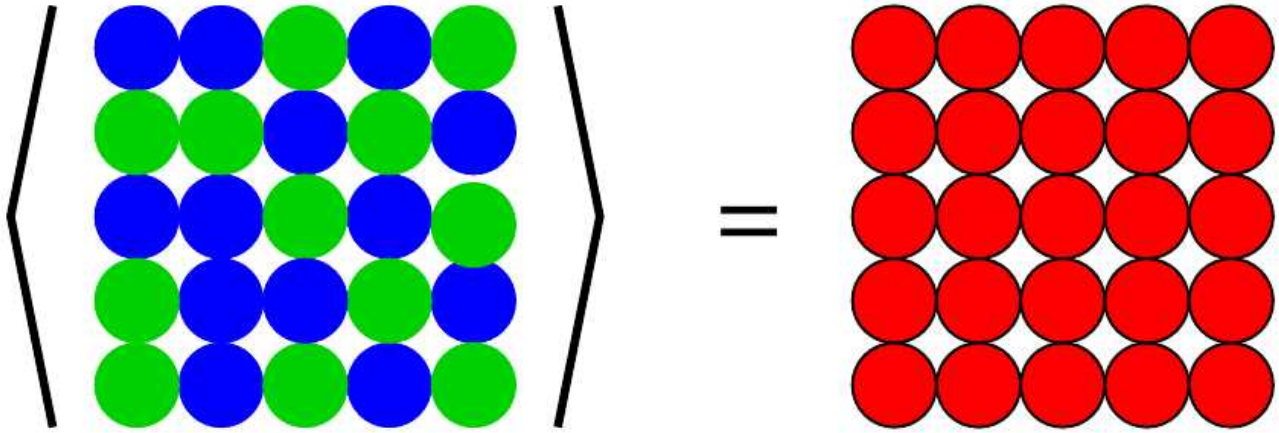
In the code

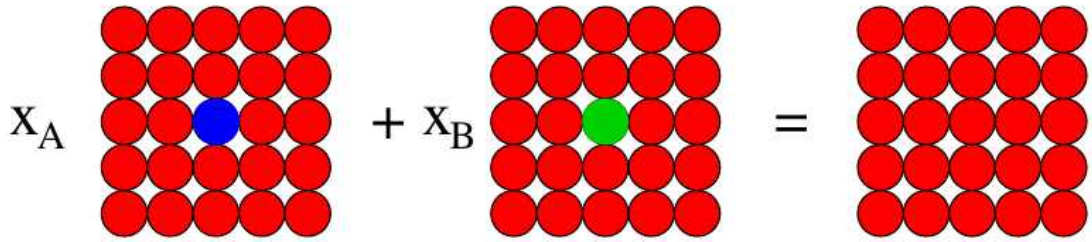
In the code

Coherent potential approximation (CPA)

Idea

find an effective CPA medium that represents the electronic structure of an configurationally averaged substitutionally random alloy $A_x B_{1-x}$

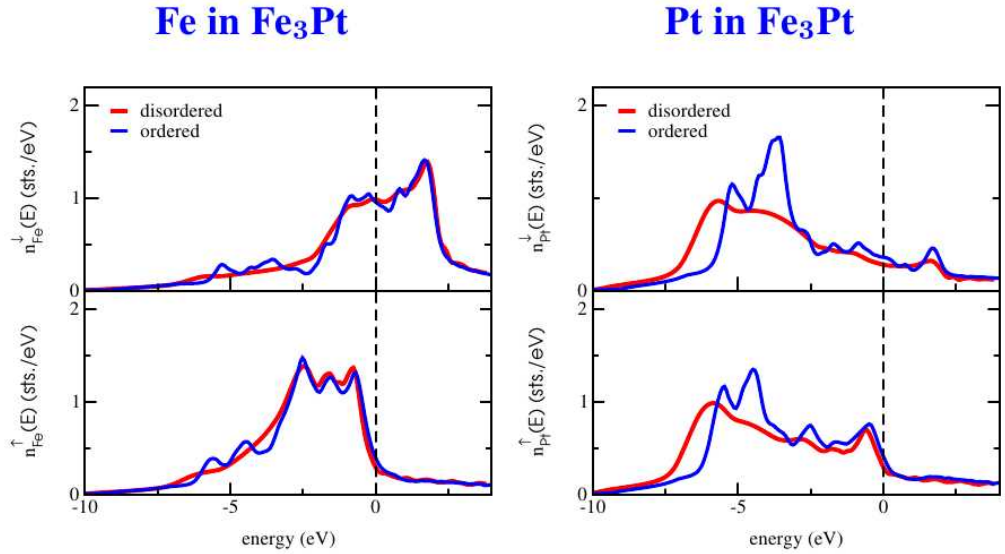




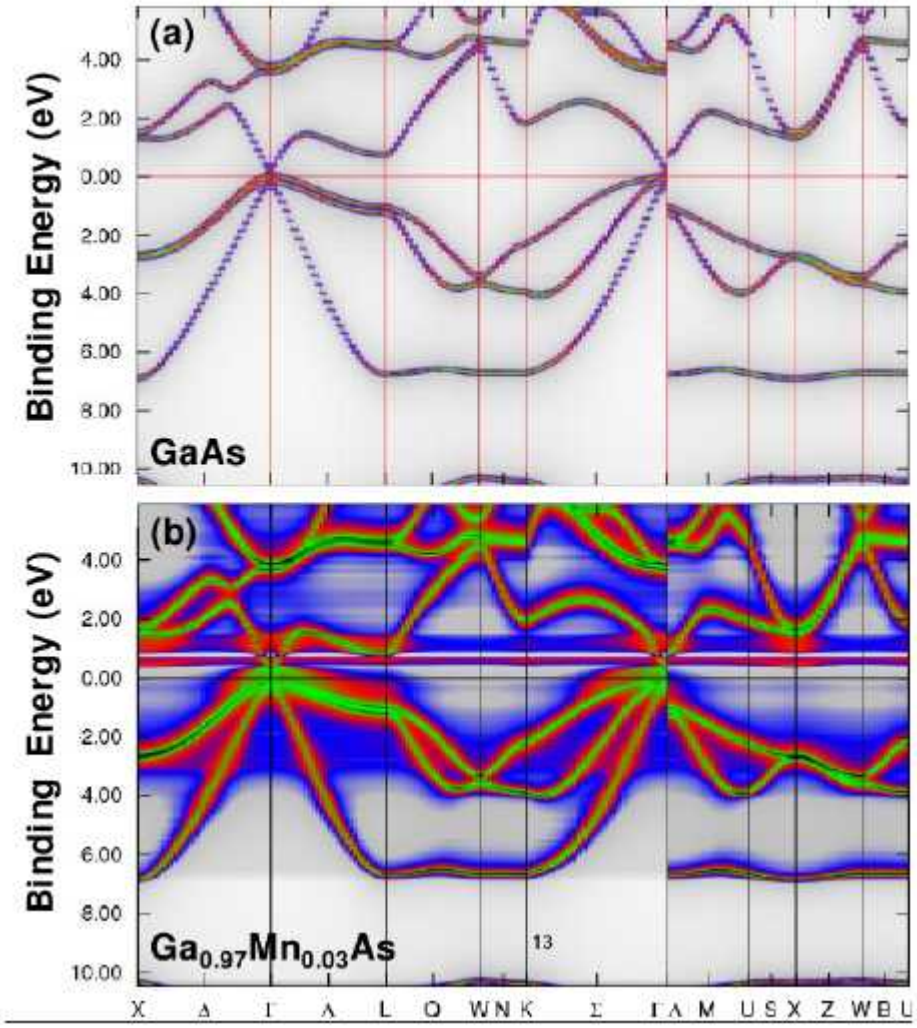
$$x_A \underline{\tau}^{nn,A} + x_B \underline{\tau}^{nn,B} = \underline{\tau}^{nn,CPA}$$

DOS and spectral functions for disordered systems

comparison of results for ordered and disordered case



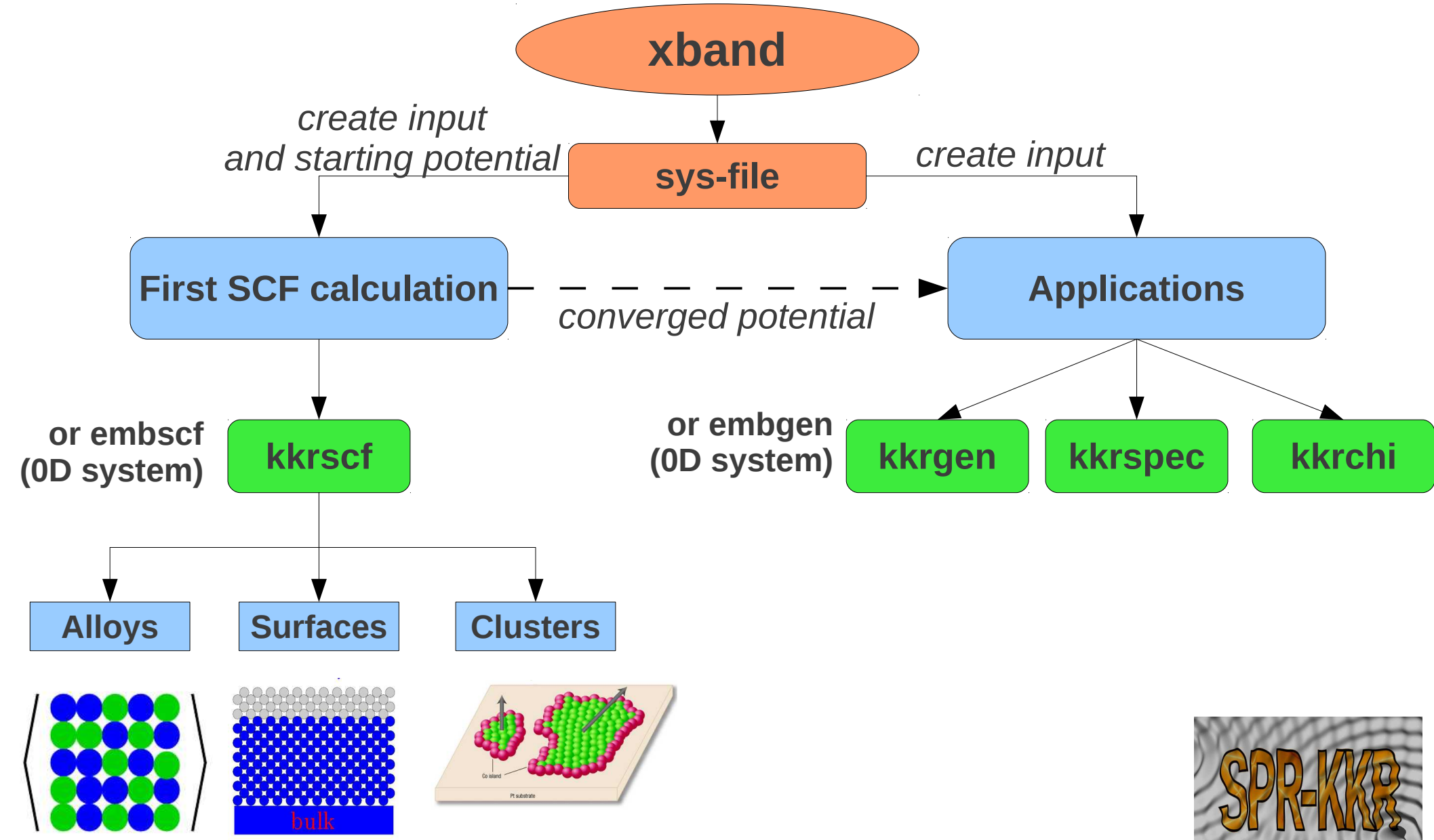
Bloch Spektralfunktion



A. Gray, J. Minar et al., Nat. Mat. **11**, 957 (2012)

Flow diagram of SPR-KKR package

Flow diagram of calculations



Self consistent calculations

kkrscf

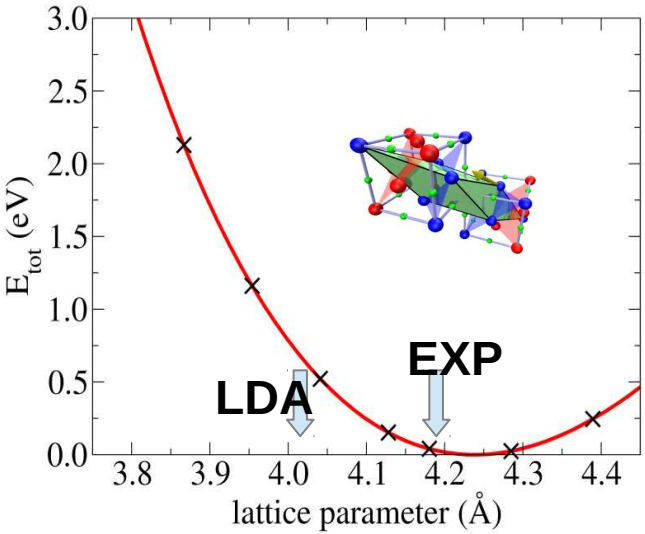
System

- Arbitrary ordered / disordered 3D, 2D systems
- 2D surfaces in TB mode
  - Semi infinite
  - Slab geometry
- Embedded clusters in 3D and 2D systems

Calculation Mode

- Spin polarized
- Scalar relativistic and fully relativistic
- Non-collinear Spin configurations
- Spin-Spirals
- SOC manipulations
- ASA and Full-potential
- LDA, GGA, LDA+*U*, LDA+DMFT (within collaboration)

Full-potential LDA+U total energy of NiO



D. Ködderitzsch et al., in preparation

Ground state and electronic properties

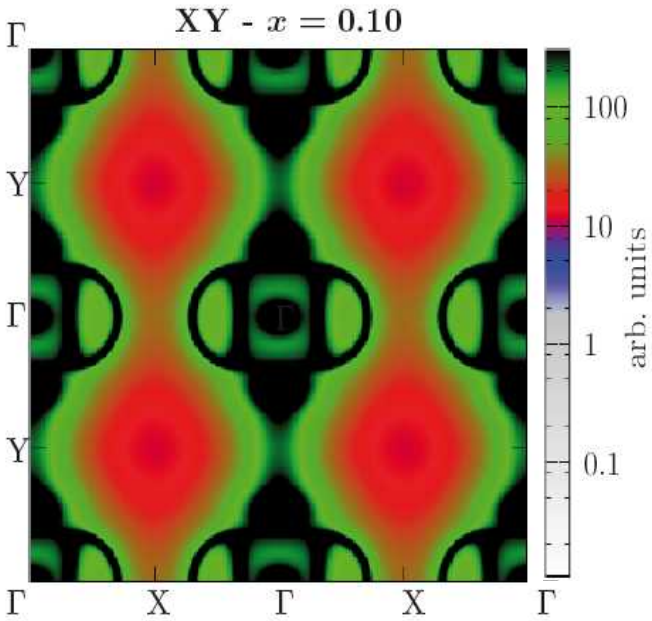
kkrgen

Ground state properties

- Spin- and orbital moments
- Magnetic form factor
- Hyperfine fields
- Exchange coupling parameters (anisotropic)

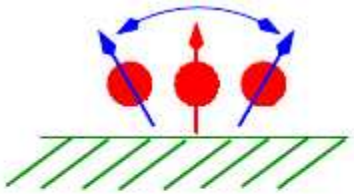
Electronic properties

- Density of states
- Dispersion relation
- Bloch spectral functions

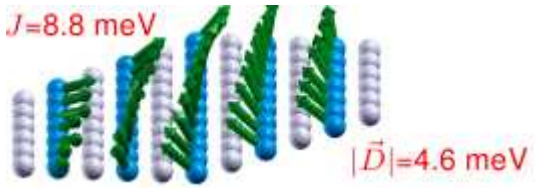


Fermi surface of $Ba(Fe_{0.9}Co_{0.1})_2As_2$

G. Derondeau et al., in preparation



$$E_x = -\frac{1}{2}\sum_{i \neq j} J_{ij}\, \hat{e}_i \cdot \hat{e}_j$$



J. Honolka et al., J. Minar et al,, PRL **102**, 067207 (2009)

Spectroscopy

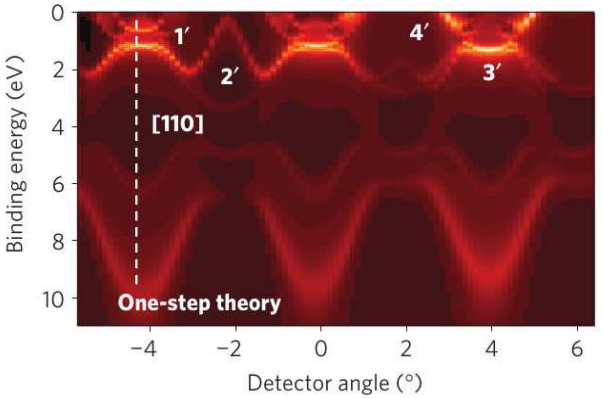
kkrgen

- X-Ray absorption + XMCD
- X-ray magnetooptics
- Magnetic compton scattering
- Positron annihilation
- AES and APS
- CL-PES

kkrspec

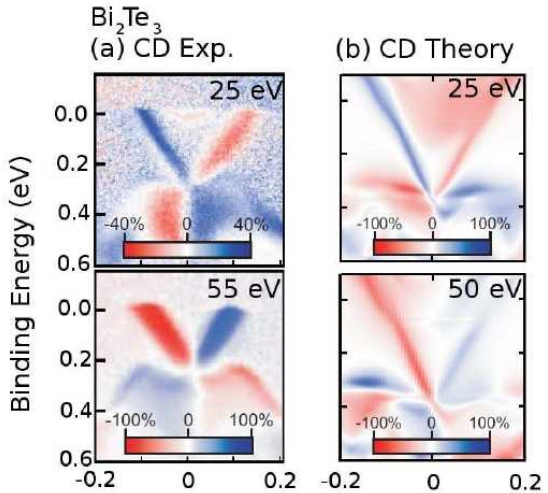
- Angle resolved PES within one-step model
- Angle integrated PES
- SP-LEED
- All calculations for:
  - Arbitrary photon energy (UV, soft X-ray, hard X-ray)
  - CPA implementation within one-step model
  - Combination with KKR+DMFT

HAXPES of W(110) at 6 keV



A. Gray et al., J. Minar et al,, Nature Materials, **10**, 759 (2011)

Topological surface states

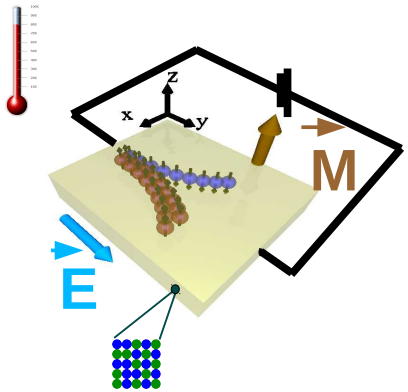


M. Scholz et al., J. Minar et al,, PRL **110**, 216801 (2013)

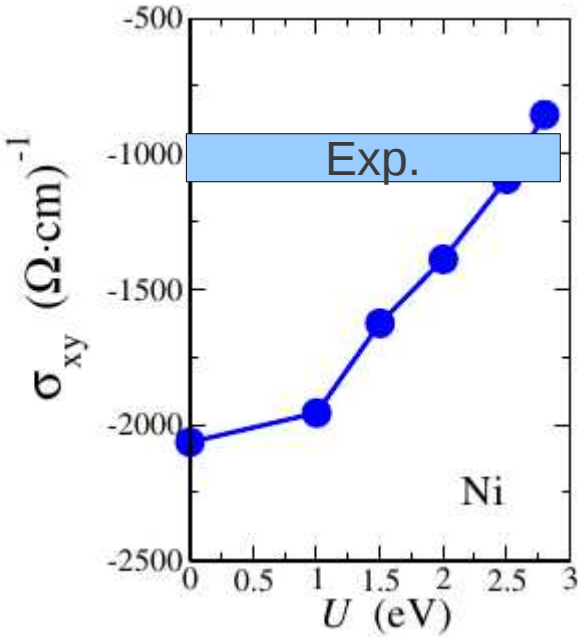
Linear response

kkrchi

- Spin and orbital magnetic susceptibility
- Gilbert damping parameters of alloys
- Conductivity: Longitudinal charge transport of alloys
- Field induced XMCD
- Knight-shift



Anomalous Hall effect of Ni



D. Ködderitzsch et al.,
New J. Phys. **15**, 053009 (2013)

Summary

The KKR-method gives

direct acces to the **Green's function**

for a description of the electronic structure

making use of **multiple scattering theory**

This central feature allows in particular to

link electronic structure and spectroscopy

in a most direct way.

More information on KKR

H. Ebert, D. Ködderitzsch and J. Minar

Calculating condensed matter properties using the KKR-Green's function method-recent developments and applications

Reports on Progress in Physics, **74**, 096501 (2011)

H. Ebert, et al.

Recent Developments in KKR Theory
Highlight of the Month" in: HCM - Newsletter of the ***k*** Network – ab initio (from electronic structure) calculation of complex processes in materials, **97**, 79 (2010)

http://www.kkr-gf.org/

Standard band structure approach III

Expectation value of operator $\mathcal{A}$

$$\langle \mathcal{A} \rangle = \sum_{j\vec{k}} \sum_{L} \sum_{L'} A_L^{j\vec{k}*} A_{L'}^{j\vec{k}} \langle R_L Y_L | \mathcal{A} | R_{L'} Y_{L'} \rangle$$

$$= \sum_{L} \sum_{L'} \underbrace{\langle R_L Y_L | \mathcal{A} | R_{L'} Y_{L'} \rangle}_{\text{operator specific matrix element}} \underbrace{\sum_{j\vec{k}} A_L^{j\vec{k}*} A_{L'}^{j\vec{k}}}_{\text{electronic structure averaged over BZ}}$$

$$= \sum_{L} \sum_{L'} \mathcal{A}_{LL'} \rho_{L'L}$$

ρ: spectral function

$$= \text{Trace } \mathcal{A} \rho$$

Lippman Schwinger equation

$\mathcal{H}_0$: Hamiltonian for unperturbed reference system

$$\begin{aligned}(E - \mathcal{H}_0)\,\Psi_0(\vec{r}, E) &= 0 \\ (E - \mathcal{H}_0)\,G_0(\vec{r}, \vec{r}\,', E) &= \delta(\vec{r} - \vec{r}\,')\end{aligned}$$

$G_0(\vec{r}, \vec{r}\,', E)$ solving inhomogeneous equation

Treatment of perturbed system $\mathcal{H} = \mathcal{H}_0 + V(\vec{r})$

$$\begin{aligned}(E - \mathcal{H})\,\Psi(\vec{r}, E) &= 0 \\ (E - \mathcal{H}_0)\,\Psi(\vec{r}, E) &= V(\vec{r})\Psi(\vec{r}, E)\end{aligned}$$

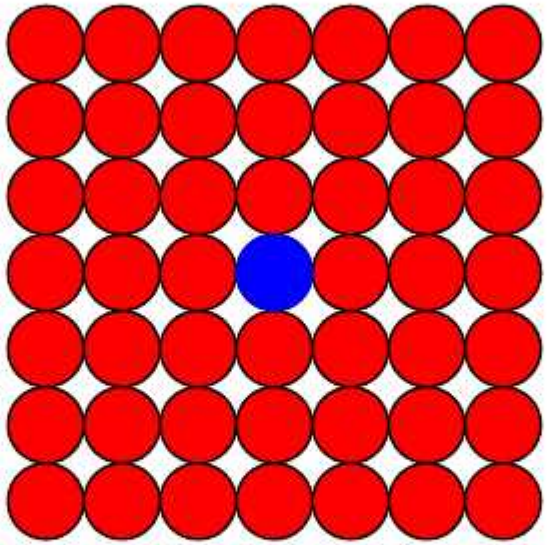
solution supplied by Lippmann-Schwinger equation

$$\Psi(\vec{r}, E) = \Psi_0(\vec{r}, E) + \int \mathrm{d}^3 r'\, G_0(\vec{r}, \vec{r}\,', E)\, V(\vec{r})\, \Psi(\vec{r}, E)$$

Substitutional impurities

Single site approximation

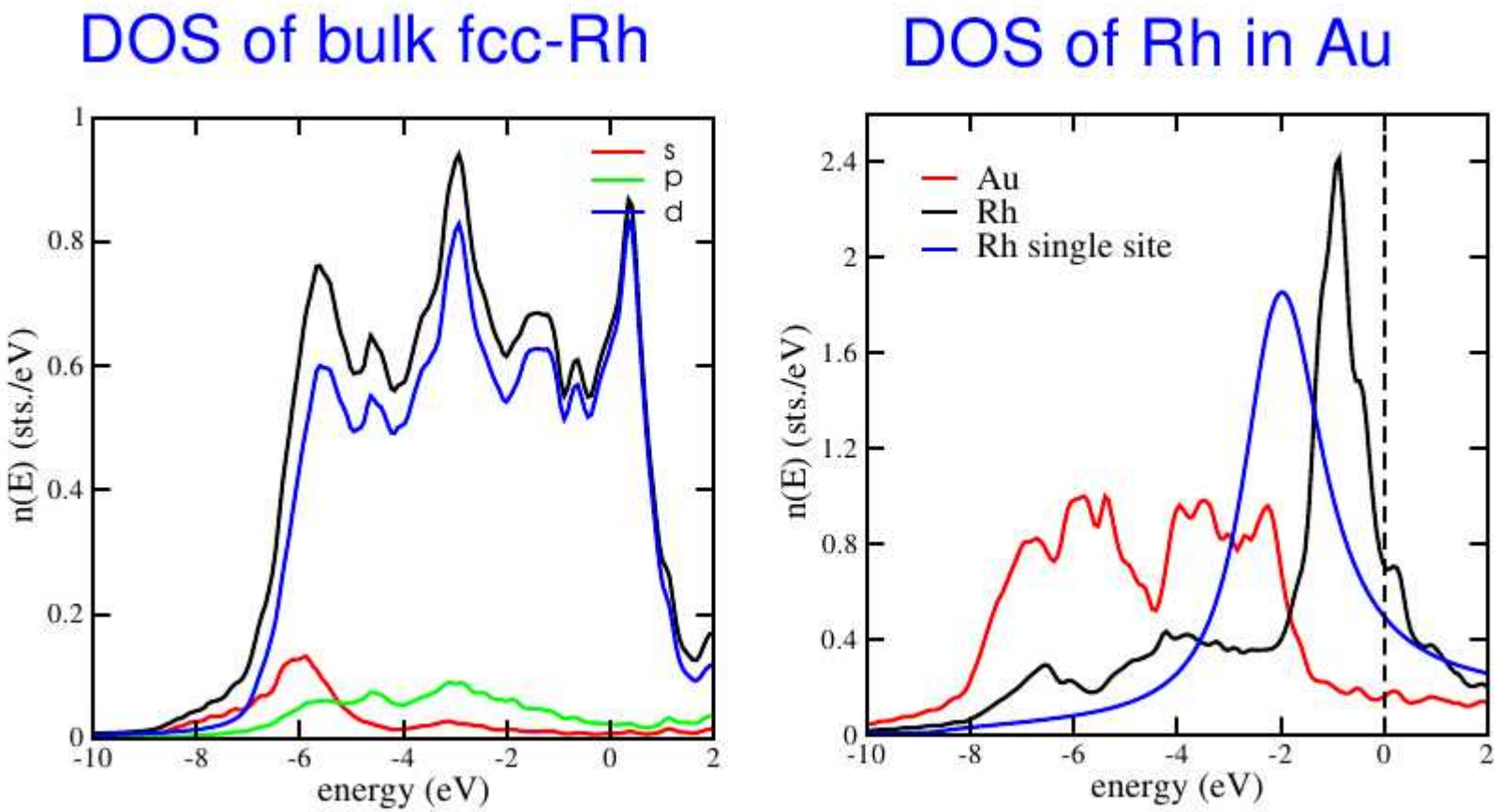
ignore the distortion of the surrounding host atoms



Assuming the impurity on site $n = 0$ one has

$$\underline{t}^n = \begin{cases} \underline{t}_{imp} & \text{for } n = 0 \\ \underline{t}_{host} & \text{for } n \neq 0 \end{cases}$$

Rh impurity in Au



Calculations:

- set concentration of impurity set to zero
- Or perform real space calculations: embedding (relaxation of electronic structure around impurity)

Single site density of states

Density of states DOS

$$n^{ss}(E) = -\frac{1}{\pi}\Im \int d^3r\, G^{ss}(\vec{r},\vec{r}',E)$$

$$= -\frac{1}{\pi}\sum_L \Im$$

$$\left[t_L(E) \int_{\Omega_n} d^3r\, Z_L^{\times}(\vec{r},E) Z_L(\vec{r},E) \right.$$

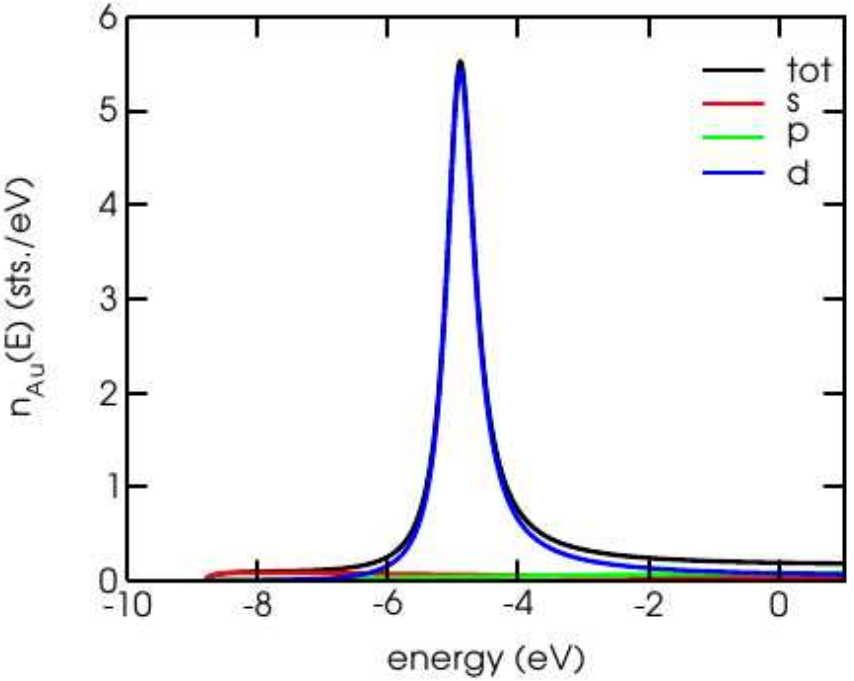
$$\left. - \int_{\Omega_n} d^3r\, J_L^{\times}(\vec{r},E) Z_L(\vec{r},E) \right]$$

for real energies

$$= -\frac{1}{\pi}\sum_L \Im\, t_l(E) \int_{\Omega_n} d^3r Z_L^{\times}(\vec{r},E) Z_L(\vec{r},E)$$

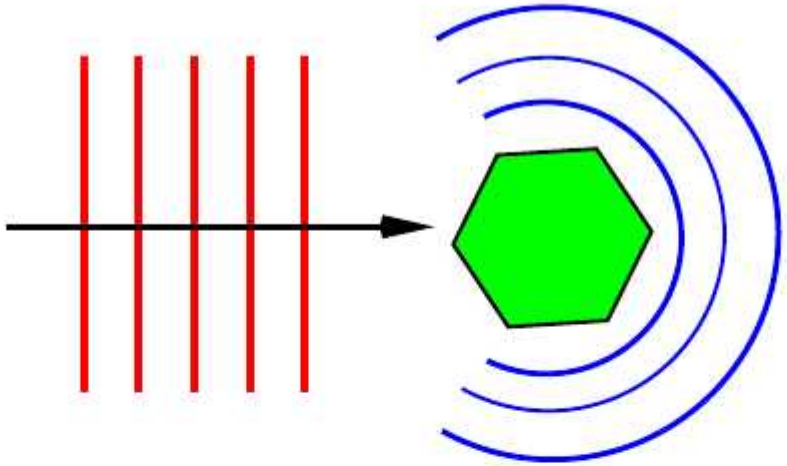
$$= n_l^{ss}(E)$$

l-resolved single site DOS $n_l^{ss}(E)$



scalar-relativistic results for Au

Standard scattering experiment



$$\psi(\vec{r}, E) = \underbrace{e^{i\vec{k}\cdot\vec{r}}}_{\text{incoming plane wave}} + f(\theta, \phi) \underbrace{\frac{e^{ikr}}{r}}_{\text{outgoing spherical wave}}$$

scattering amplitude $f(\theta, \phi)$