Modeling of materials, where we were, where we are and where we are going

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Overview

Some early calculations, what one could do

Current research projects

- DMFT
- Finite temperatures
- Dynamics
- ‘new’ systems
- an automatic modeling mashinery

Perspectives

Symmetrized Relativistic Augmented-Plane-Wave Method: Gray Tin and the Warped Muffin-Tin Potential*

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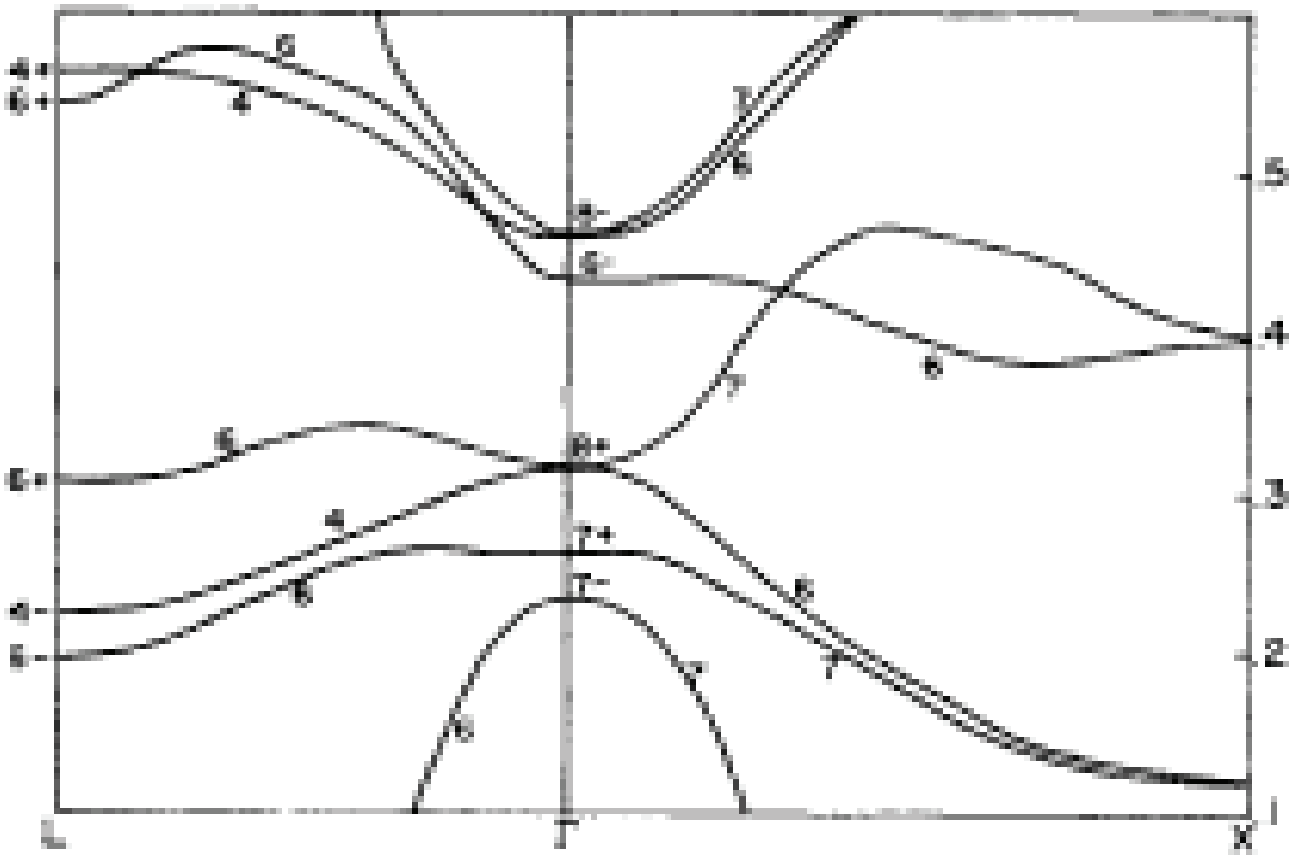
and
Magnetic Theory Group, Physics Department, Northwestern University, Evanston, Illinois 60201
(Received 30 June 1969)



Slater exchange
not self-consistent

Anisotropic g Factors of Nickel, Palladium, and Platinum*

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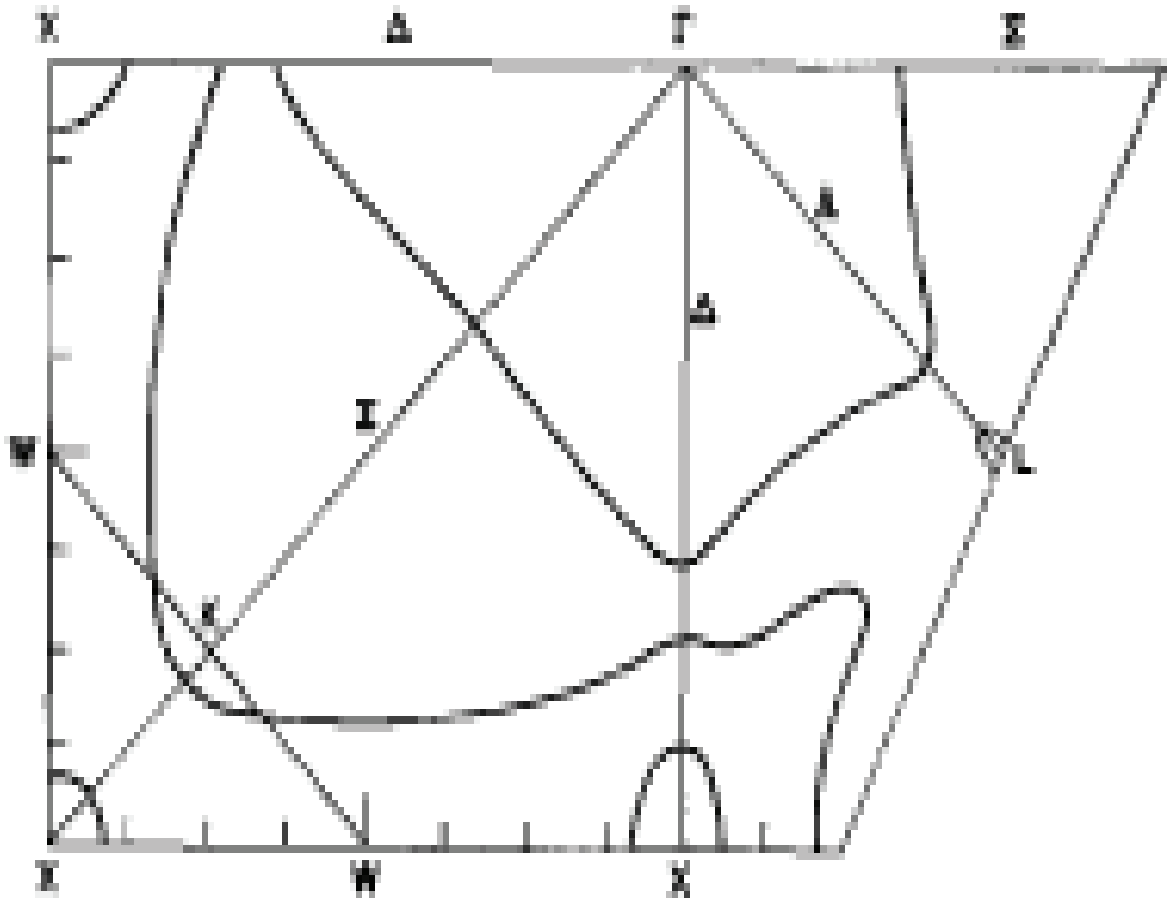
Fermi surface of Pd



Density functional Theory

$$\left(\frac{-\Delta}{2} + V_{LSDA}\right)\psi = \varepsilon\psi$$

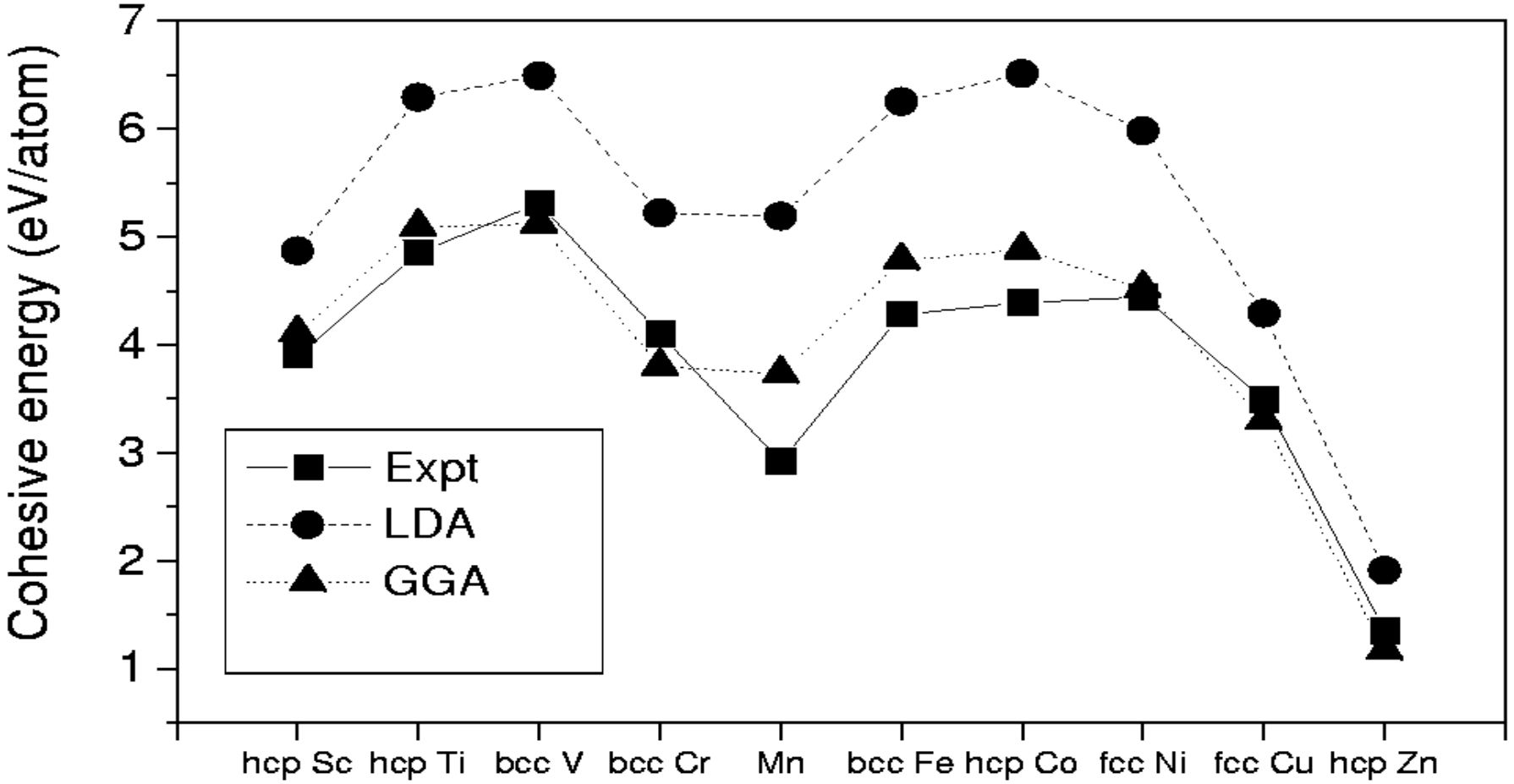
$$V_{LSDA}(n(r))$$

$$n(r) = \sum \psi(r)^2$$

$$E(n(r)) \longrightarrow$$

density
elasticity
magnetism
structure
stability

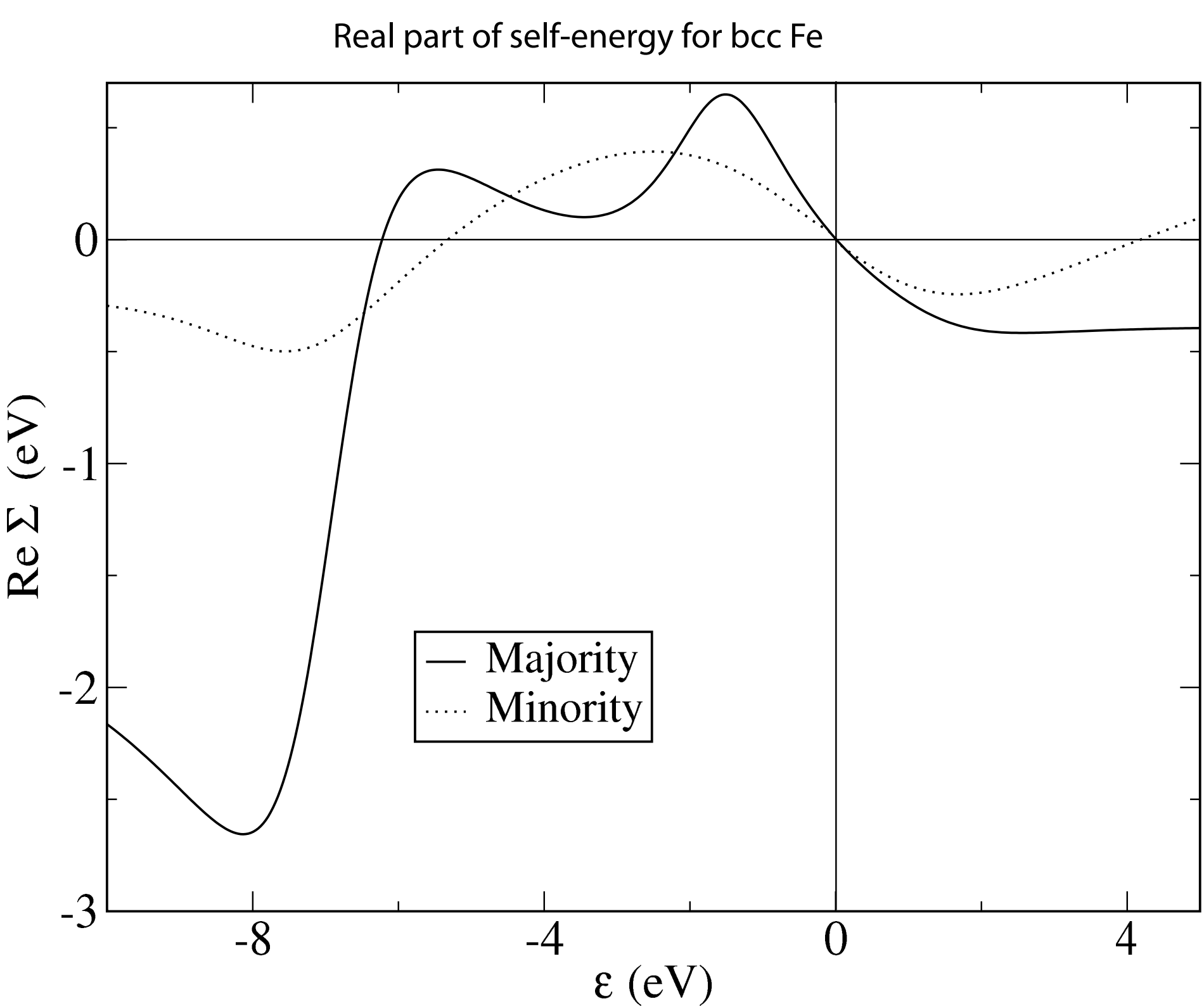
Cohesive energy of 3d elements; LSDA vs. GGA



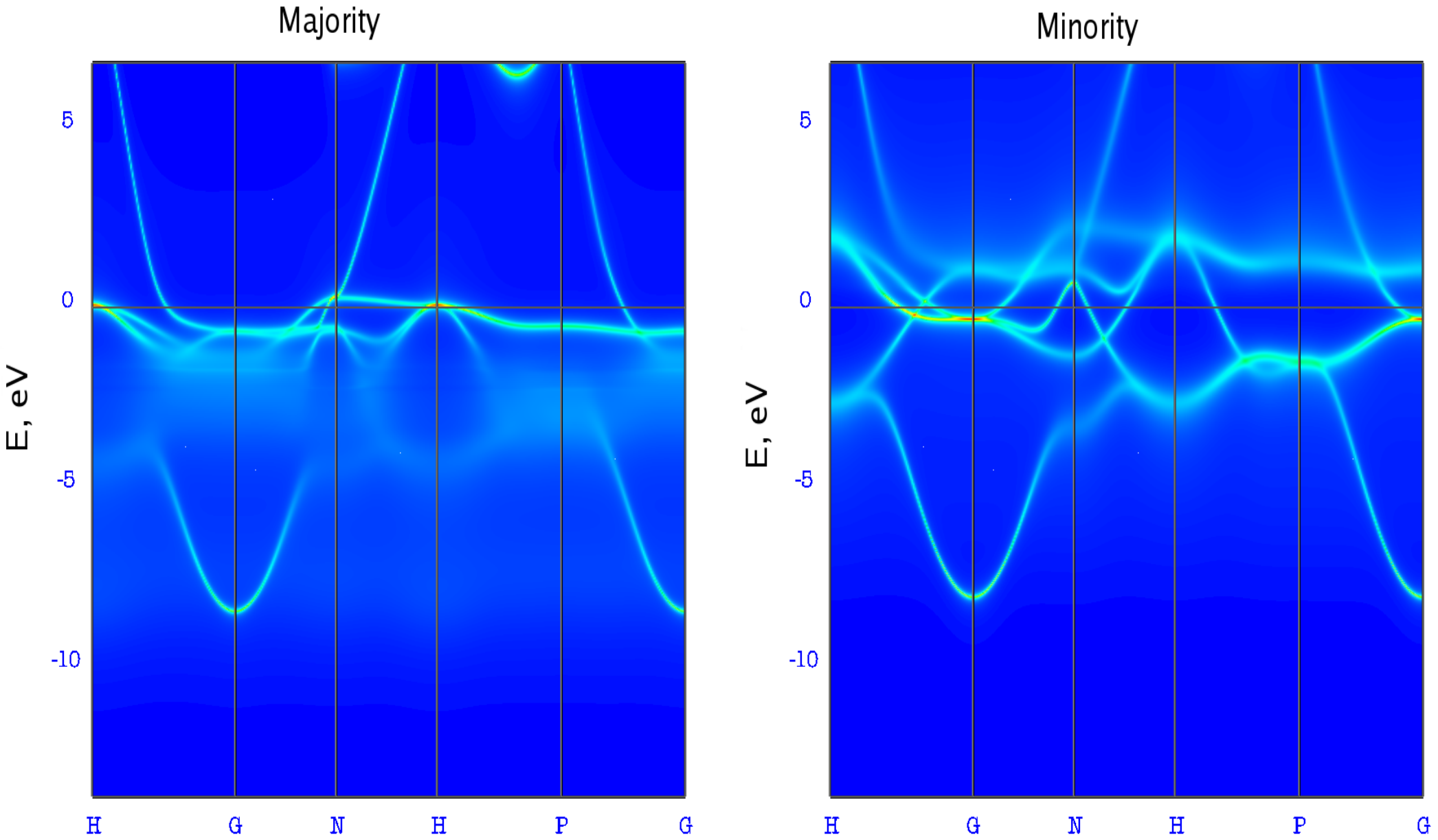
Improving on the effective potential

$$G(z) = [(z - \mu) - h_{LSDA} - \Sigma(z)]^{-1}$$

$\Sigma(z)$ the self-energy, which adds interactions normally not included in LSDA or GGA (i.e. Hubbard U). It can be calculated as an impurity problem in the dynamical mean field theory


Real part of self-energy for bcc Fe
0
-1
-2
-3
Re Σ (eV)
-8
-4
0
4
ε (eV)
Majority
Minority

Energy ‘bands’ of bcc Fe



1) Supercell method (Direct method)

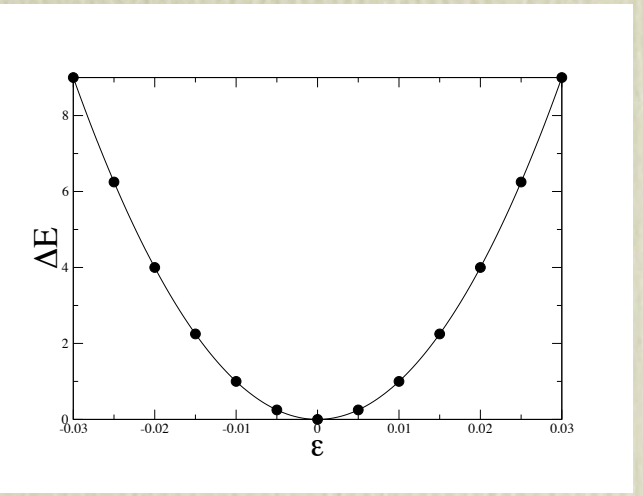
$$\mathbf{R} = \mathbf{R}_0 + \mathbf{U}_\mathbf{R} \quad \Rightarrow \quad \mathbf{F}_\mathbf{R} = \langle\Psi|\frac{\partial\mathcal{H}}{\partial\mathbf{R}}|\Psi\rangle = \sum_{R'} \bar{\bar{\Phi}}(\mathbf{R}-\mathbf{R}')\mathbf{U}_{\mathbf{R}'}$$

$$\bar{\bar{D}}(\mathbf{k}) = \frac{1}{M}\sum_R \bar{\bar{\Phi}}(\mathbf{R})e^{-i\mathbf{R}\mathbf{k}} \quad \Rightarrow \quad \omega_{\mathbf{k}s} \quad , \quad \epsilon_{\mathbf{k}s}$$

2) Frozen phonon calculation

$$\mathbf{R} = \mathbf{R}_0 + \epsilon\epsilon_{\mathbf{k}s} sin(\mathbf{k}\mathbf{R}_0)$$

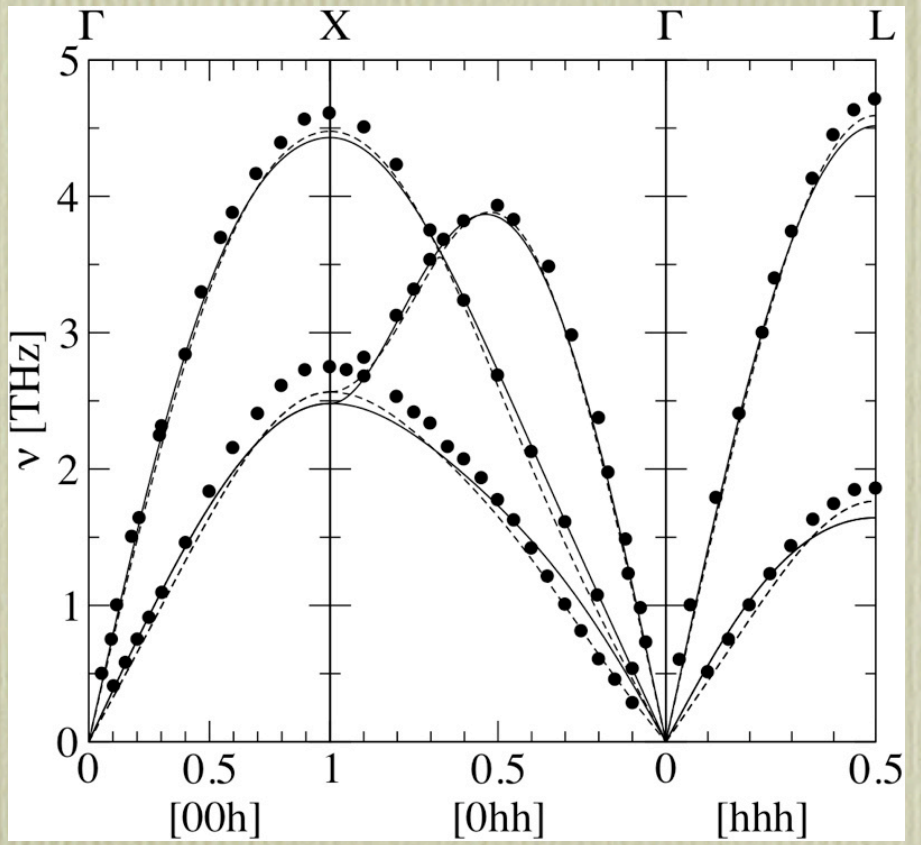
$$\Rightarrow \quad \omega_{\mathbf{k}s} = \sqrt{\frac{1}{M}\frac{\partial^2\Delta E}{\partial\epsilon^2}}$$

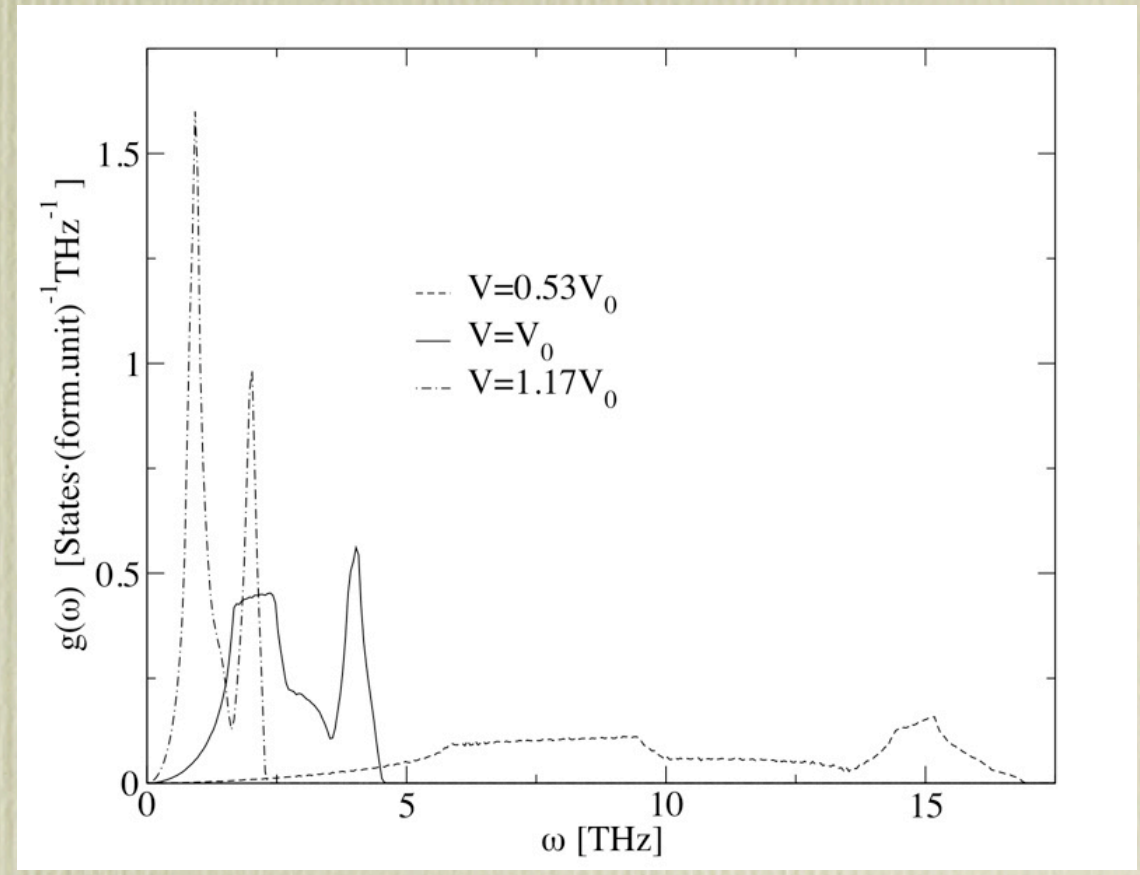


3) Linear response

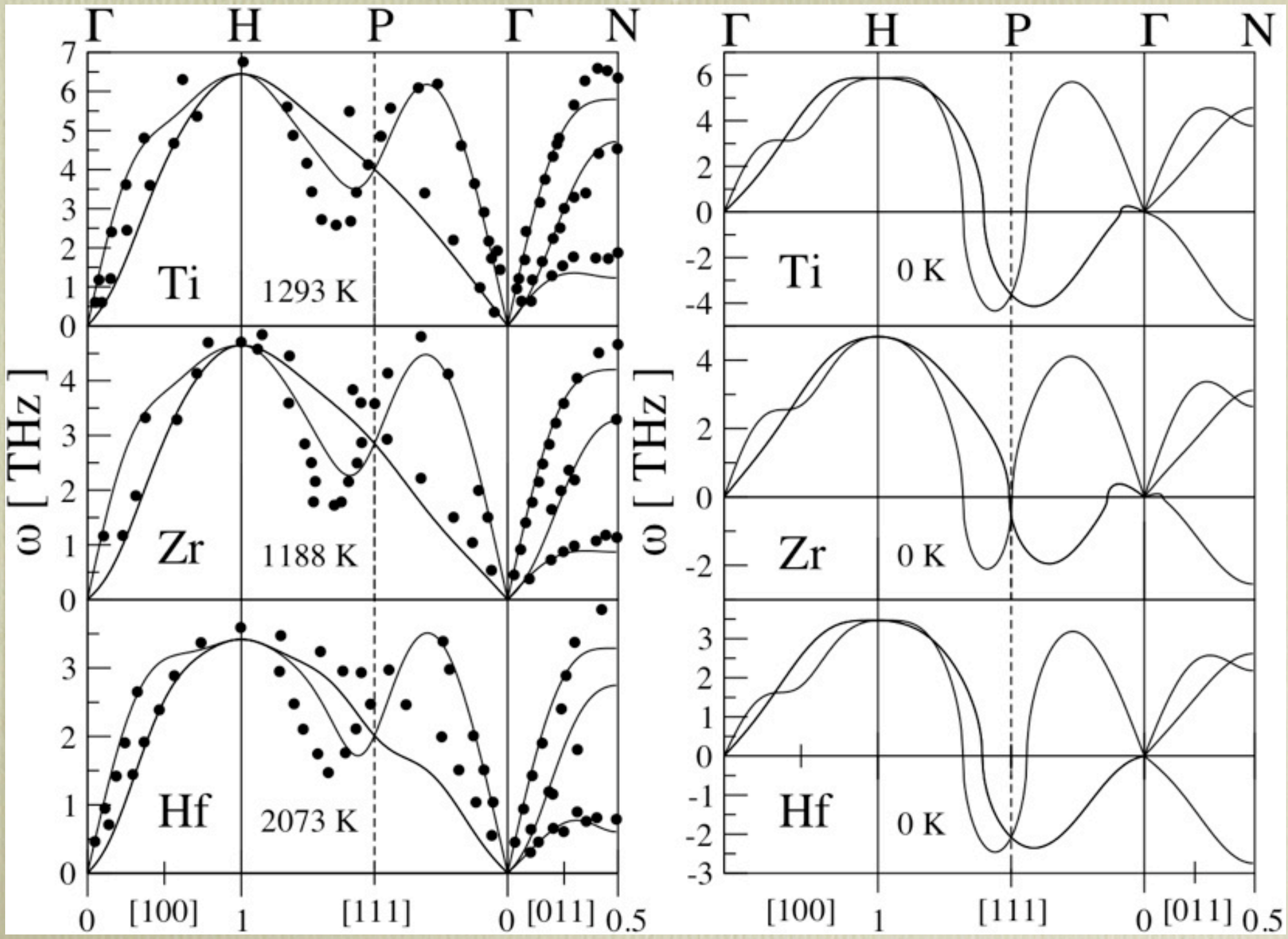
Results (paper III)

FCC Au





Results (paper VI)



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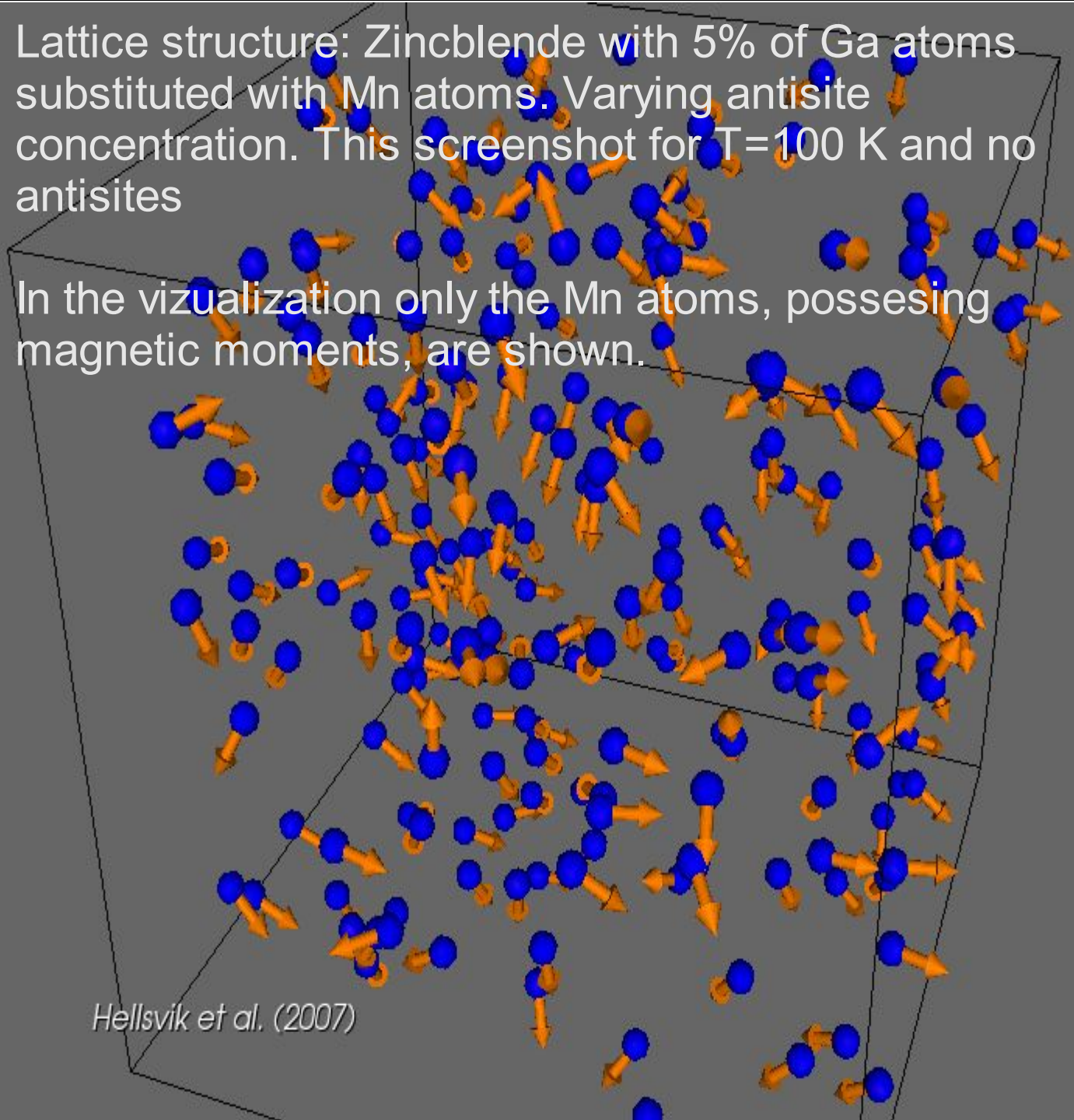
Lattice structure: Zincblende with 5% of Ga atoms substituted with Mn atoms. Varying antisite concentration. This screenshot for T=100 K and no antisites

In the vizualization only the Mn atoms, possesing magnetic moments, are shown.



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Equations of motion: Atomistic Landau-Lifshitz-Gilbert eq.

$$\frac{d\mathbf{m}_i}{dt} = -\gamma[\mathbf{m}_i \times [\mathbf{B}_i + \mathbf{b}_i(t)]] - \gamma\frac{\alpha}{m}[\mathbf{m}_i \times [\mathbf{m}_i \times [\mathbf{B}_i + \mathbf{b}_i(t)]]]$$

Precession term

Damping term

Derived from spin-polarized KS-Hamiltonian, using a separation of time-scales, following Antropov et al, PRB **54**, 1019 (1996).

γ Gyromagnetic ratio

α damping parameter

$$\frac{\partial \hat{\mathbf{S}}}{\partial t} = \frac{1}{i\hbar}[\hat{\mathbf{S}}, \mathscr{H}_{\mathrm{KS}}]$$

$$\mathbf{B}_i = -\frac{\partial \mathscr{H}}{\partial \mathbf{m}_i}$$

Magnetic exchange is mapped onto a Heisenberg hamiltonian

$$\mathscr{H}_{\mathrm{ex}} = -\frac{1}{2}\sum_{i \neq j} J_{ij}\mathbf{m}_i \cdot \mathbf{m}_j$$

The details of our method are described in detail in the PhD thesis of Björn Skubic (Sep 2007).

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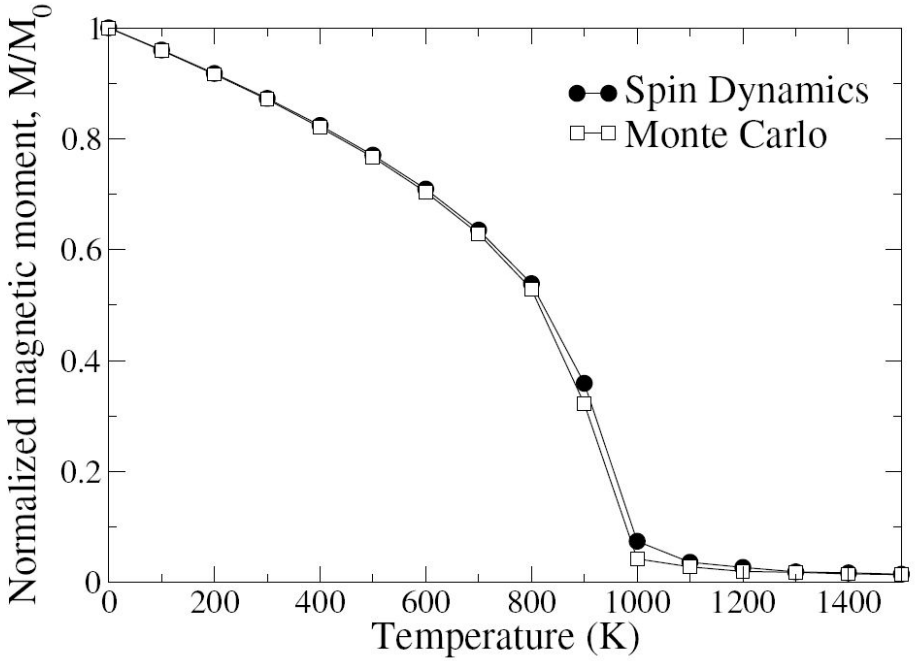
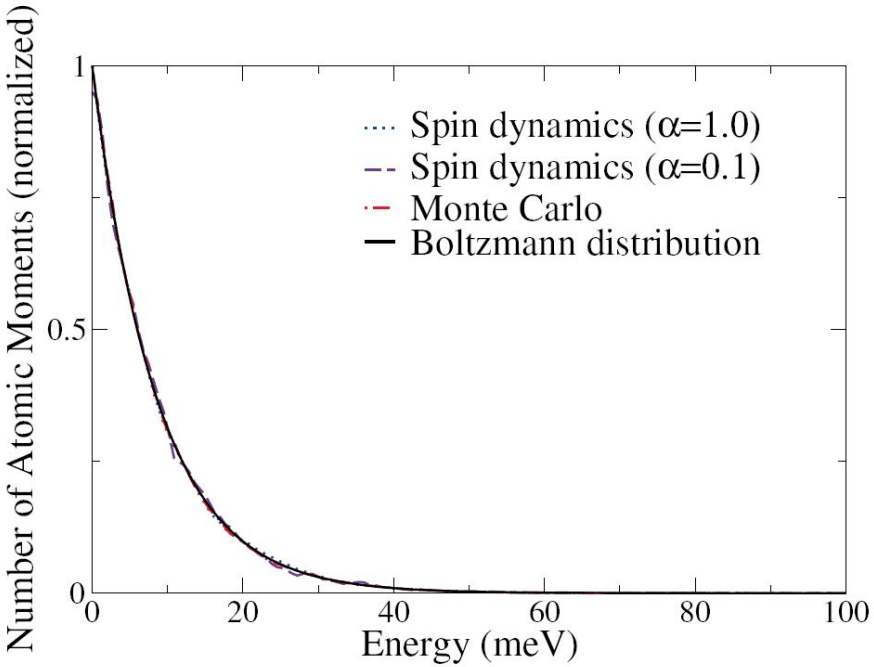
The ensemble average of the magnetization

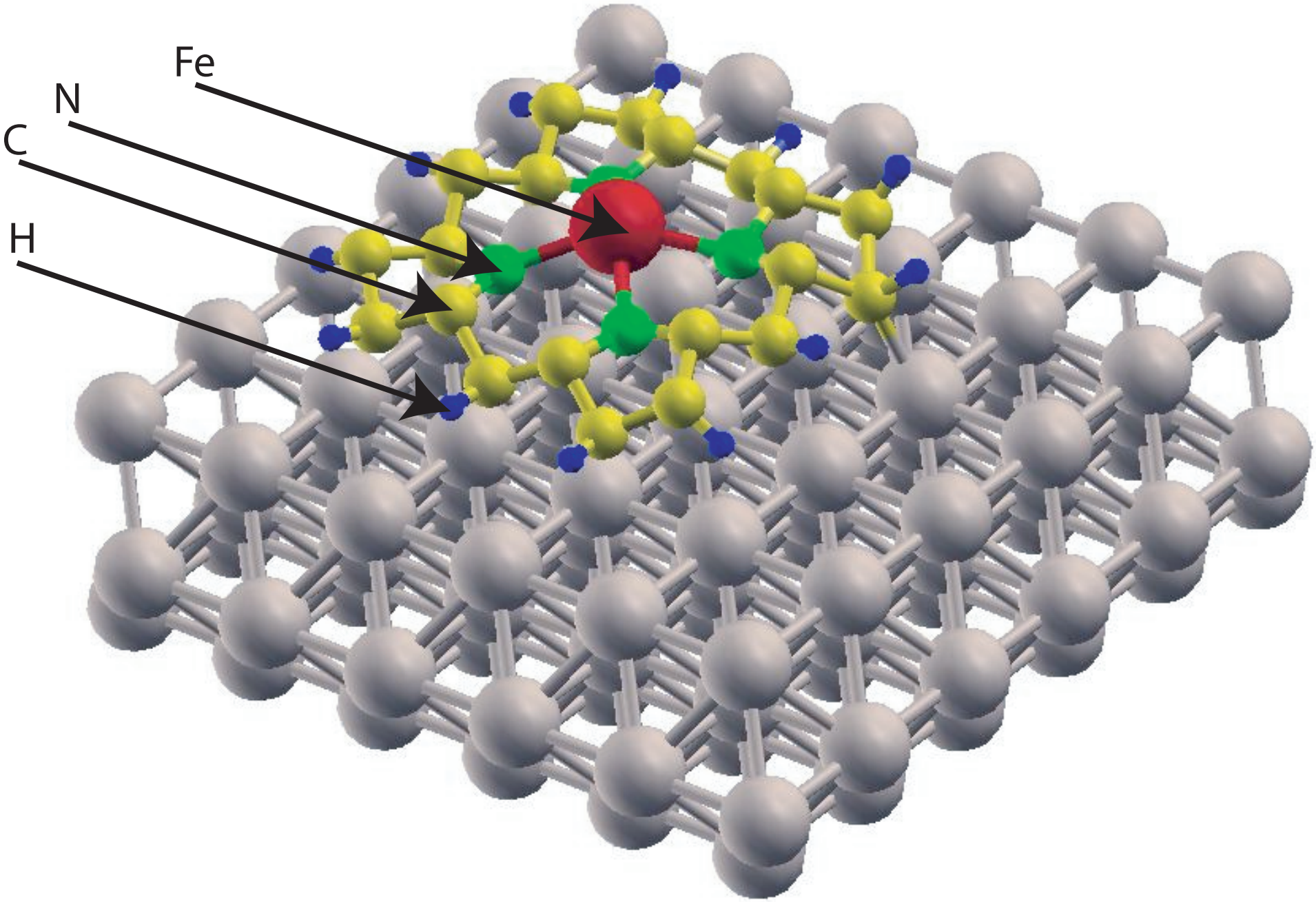


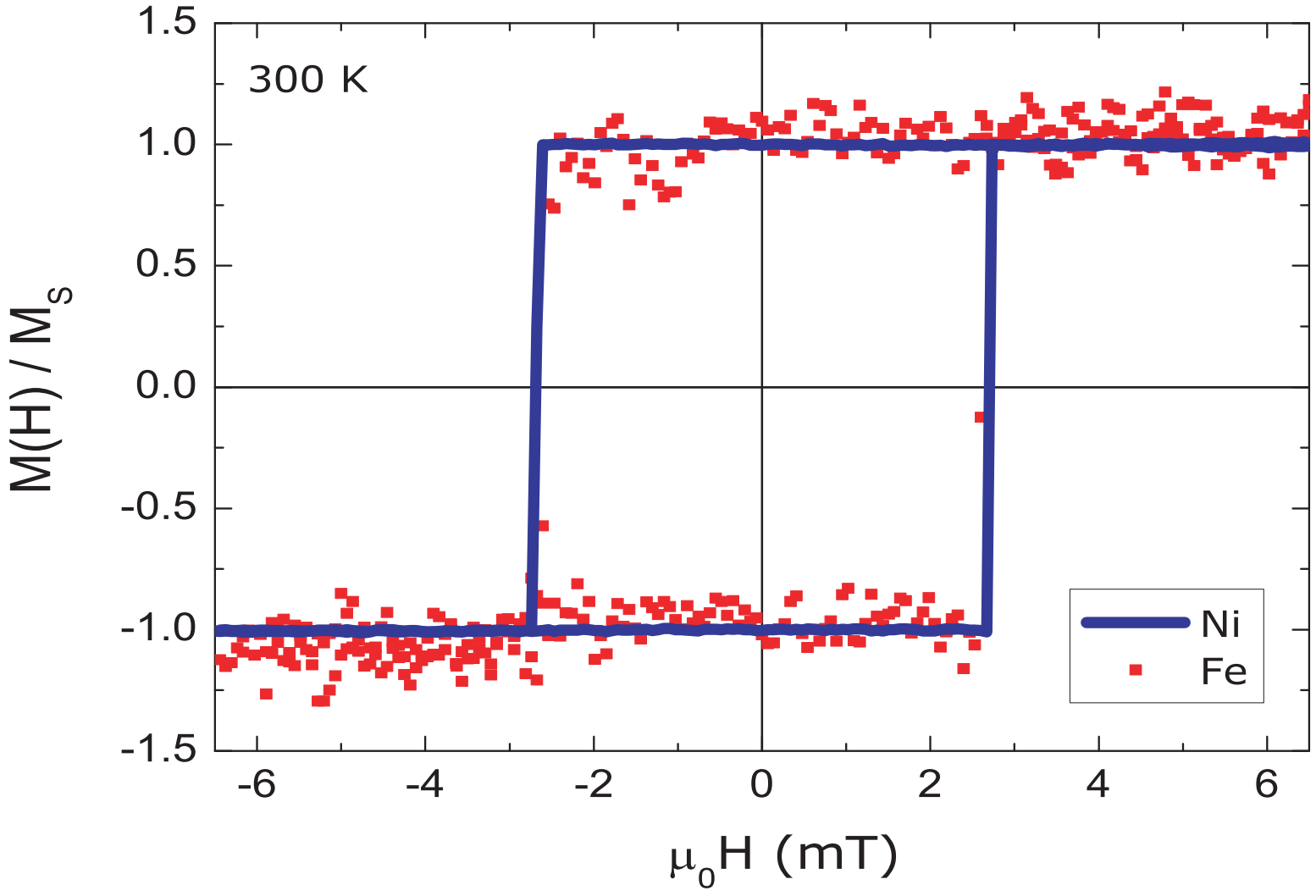
The equilibrium configurations conform with those obtained in Monte Carlo simulations.



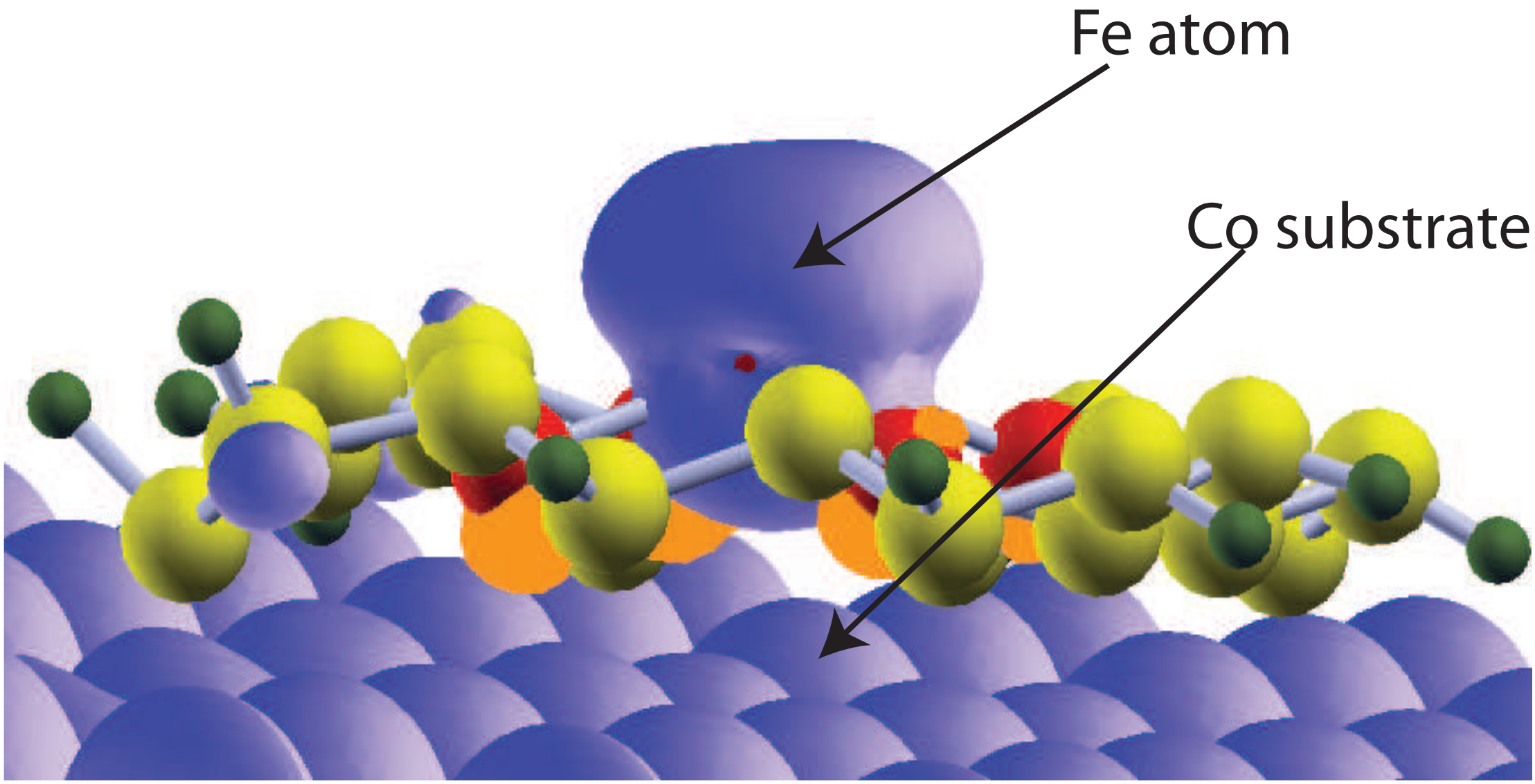
The distribution of magnetic moment energies

Structural property of porphyrine on Co/Ni



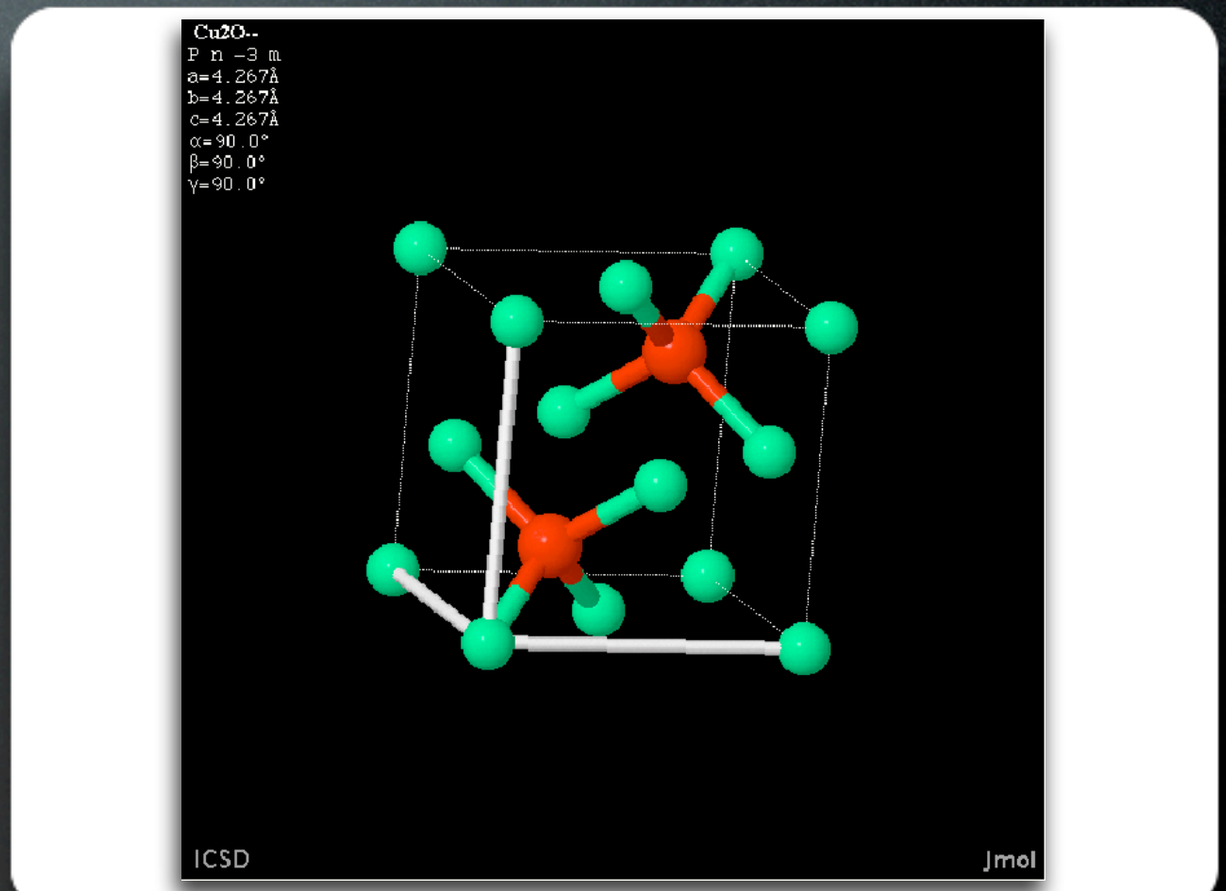

300 K
M(H) / M_S
μ_0H (mT)
Ni
Fe
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-6
-4
-2
0
2
4
6

Magnetisation density around Fe-porphyrine and Co surface (red=N atom, yellow=C atom, green = C atom)



Inorganic Crystal Structure Database

- http://icsd.ill.fr/icsd/index.html
- Crystal structure data since 1913
- 97376 entries
- View (Jmol) or export atom positions (Crystal Maker)



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IO      SHOW=t  HELP=F  WKP=F  VERBOS=41 30  IACTIVE=f
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SYMGRP  find
BZ      NKABC=16 16 16  METAL=F  TOL=1.D-4  TETRA=T
        NPTS=1500  SAVDOS=T
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         EREF=-14220.826416
         RSMH= 3.094 1.774 EH= -0.664 -0.172
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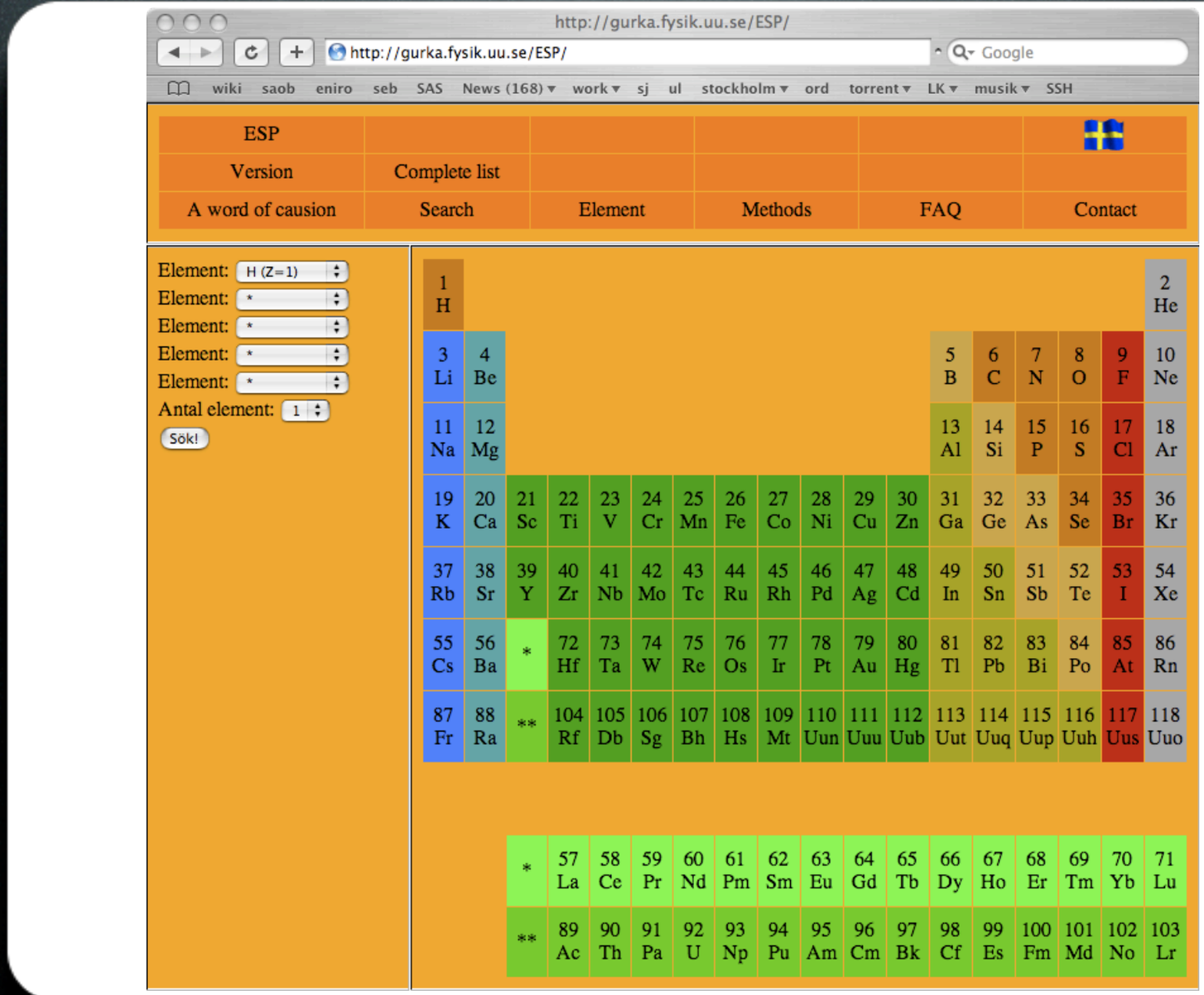
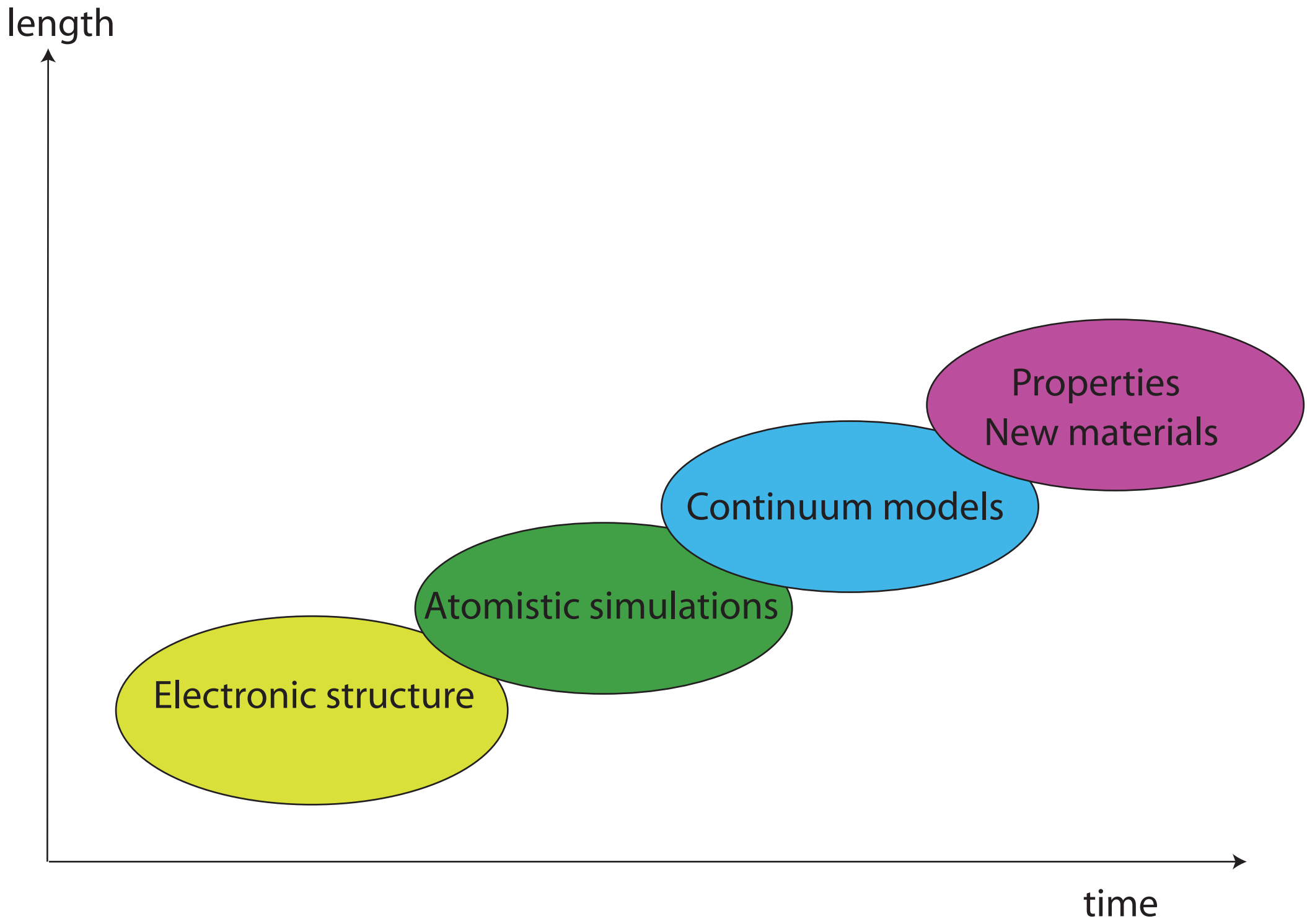
Control file for LMTO



Electronic Structure Project


length
Properties
New materials
Continuum models
Atomistic simulations
Electronic structure
time