All-Electron Full-Potential Calculations at $\mathcal{O}$(ASA) Speed — A Fata Morgana?

Volker Eyert

SFB 484, Teilprojekt D6

October 5, 2007

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Outline

1 Background

2 Full-Potential ASW Method

3 Proof of Concept: Results

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2. Full-Potential ASW Method
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Back in the 1930's . . .

John C. Slater

Full Potential

$$v_\sigma(\mathbf{r}) : \begin{cases} \text{spherical symmetric near nuclei} \\ \text{flat outside the atomic cores} \end{cases}$$

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Muffin-Tin Approximation

$$v_\sigma^{MT}(\mathbf{r}) = \begin{cases} \text{spherical symmetric in spheres} \\ \text{constant in interstitial region} \end{cases}$$

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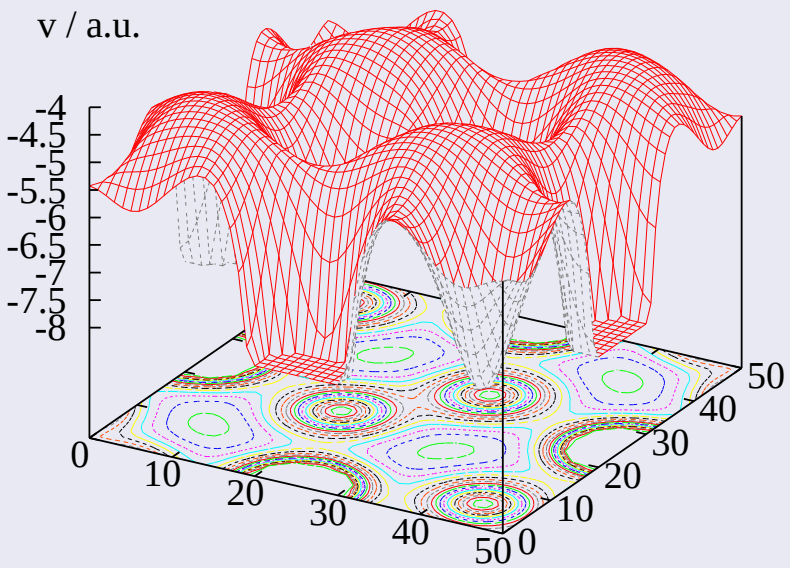
Full Potential (FeS_2)



Muffin-Tin Potential

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Muffin-Tin Approximation

distinguish:

- atomic regions
- remainder

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distinguish:

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Muffin-Tin Potential

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Partial Waves

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    - plane waves
    - spherical waves

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Basis Functions

- matched partial waves
  - augmented plane waves (APWs)
  - „muffin-tin orbitals" (MTOs), augmented spherical waves (ASWs)

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Wave Function

expand in basis functions

- expansion coefficients from variational principle

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Core States

all-electron methods

- fully included
- orthogonal to partial waves

Basis Functions

- matched partial waves
  - augmented plane waves (APWs)
  - „muffin-tin orbitals" (MTOs), augmented spherical waves (ASWs)
- used to describe valence states

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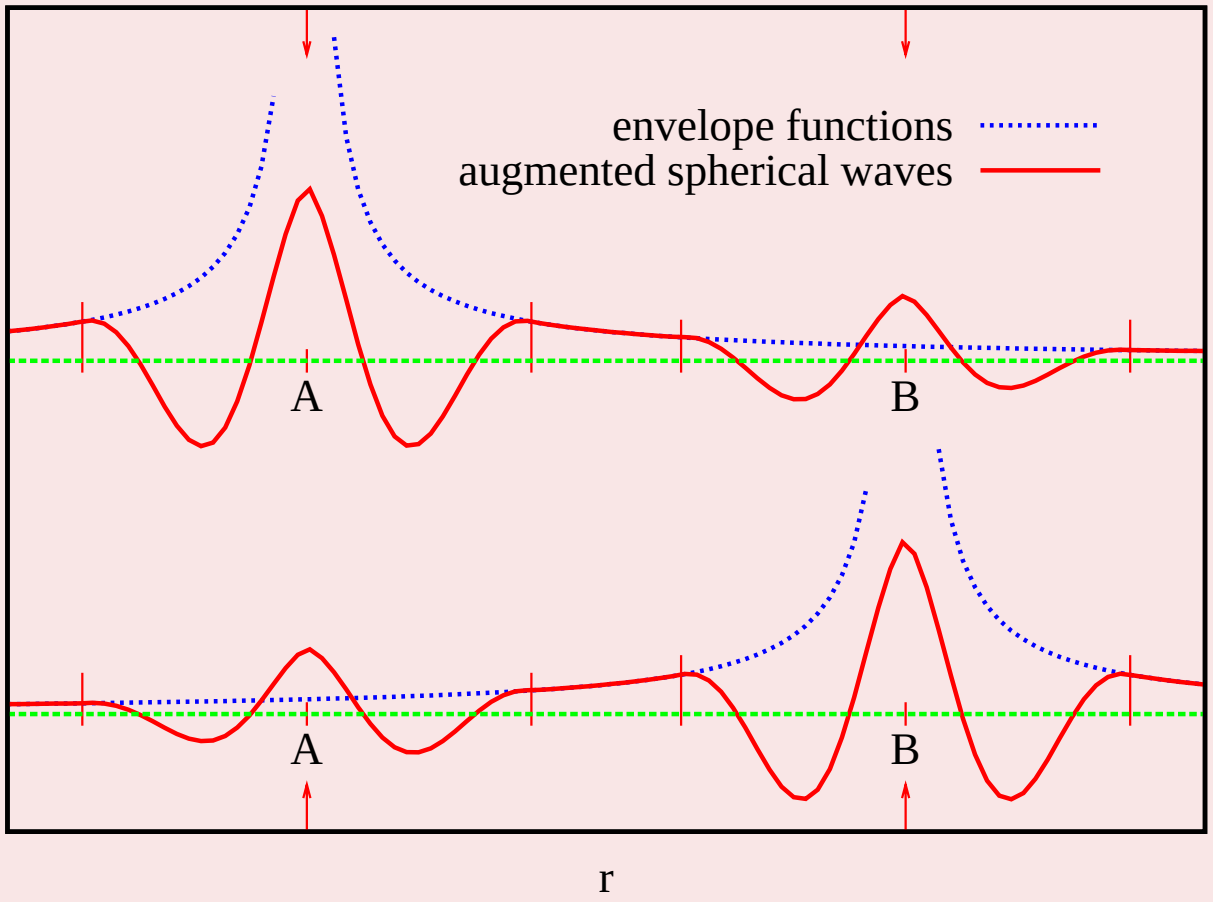
Augmented Spherical Waves



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Ole K. Andersen

"Linear Methods in Band Theory"

- energy dependence of basis functions almost linear $\rightarrow$ linearize $(\varphi, \dot{\varphi})$
  - huge increase in computat. efficiency!

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Linear Augmented Plane Wave (LAPW)

- muffin-tin approximation
- easy to implement — good!
- full-potential at a low price
  - basis functions from muffin-tin potential
  - wave functions from full potential
  - example: Wien2k
- large basis set ($\approx$ 100 pw's/atom) — bad!

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Linear Muffin-Tin Orbital (LMTO)

- based on spherical waves
  - does not require crystalline periodicity
  - natural interpretation of results
- difficult to implement bad!
- full-potential extension extremely difficult
- muffin-tin approximation (?)
  - finite interstitial region
  - large basis set:
    two functions per s-, p-, d-state
  - still inefficient bad!

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  - make spheres space-filling!
    - interstitial region formally removed
    - only numerical functions in spheres
  - minimal basis set (s, p, d)
    - very high computational efficiency
      $\rightarrow \mathcal{O}$(ASA) speed!!!
  - makes potential more realistic
  - systematic error in total energy bad!

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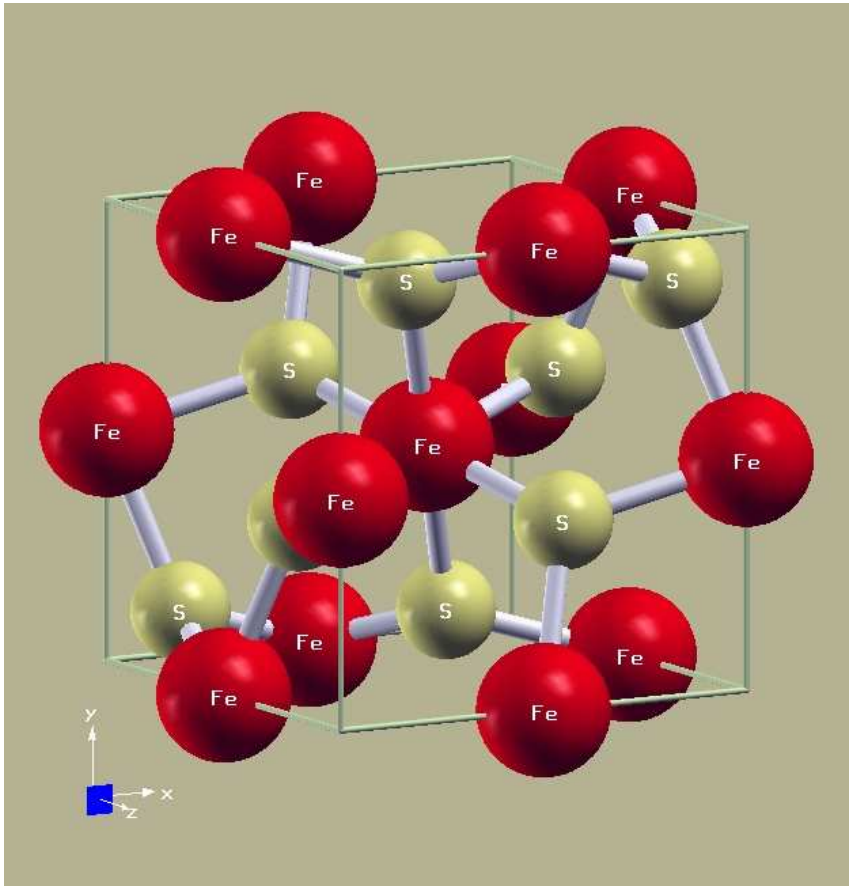
Iron Pyrite: FeS_2



Pyrite

- $Pa\bar{3}$ (T_h^6)
- a = 5.4160 Å
- "NaCl structure" sublattices occupied by
  - iron atoms
  - sulfur pairs
- sulfur pairs $\parallel \langle 111 \rangle$ axes
- x_S = 0.38484
- rotated FeS_6 octahedra

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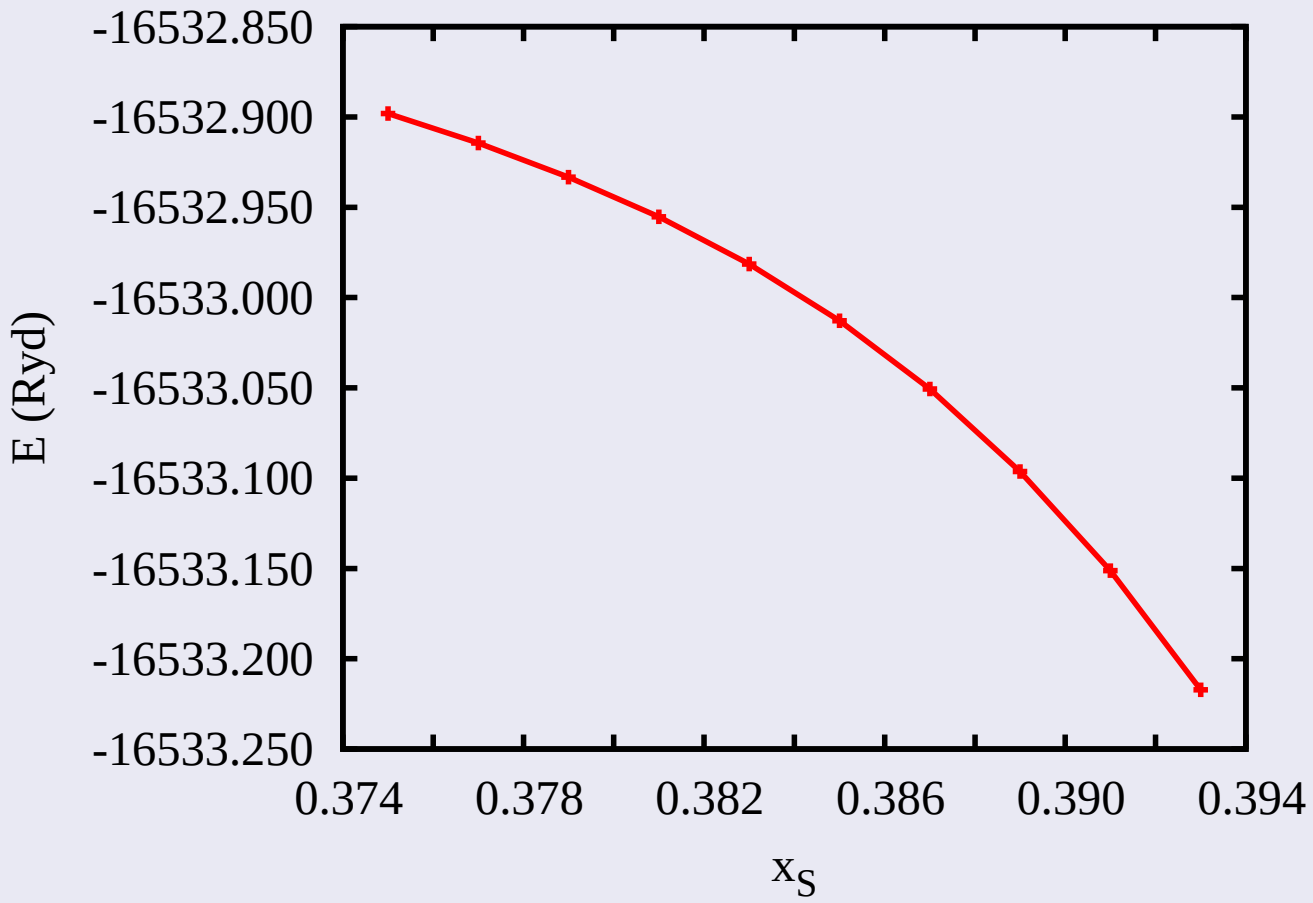
FeS_2: Structure Optimization

ASW Version 2.2



Towards a Full-Potential Spherical-Wave Method

Conclusions

- ASA (space-filling atomic spheres)
  - $\mathcal{O}$(ASA) speed
  - systematic error in total energy
- non-overlapping muffin-tin spheres
  - prerequisite for accurate total energies
  - larger basis set $\rightarrow$ inefficient

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Requirements

- restore interstitial region
  - go to non-overlapping muffin-tin spheres
  - go beyond constant-potential approximation
- inside muffin-tin spheres
  - non-spherical contributions

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Guidelines

- interstitial quantities expanded in plane waves
  - straightforward to implement
  - inefficient
- interstitial quantities expanded in spherical waves
  - elegant, no periodicity required
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  - difficult to implement

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ASW Method

Characteristics

- similar to LMTO
  - different linearization scheme
  - different interstitial energy
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0th Generation (Williams, Kübler, Gelatt, 1970s)

PRB **19**, 6094 (1979)

ASW Method

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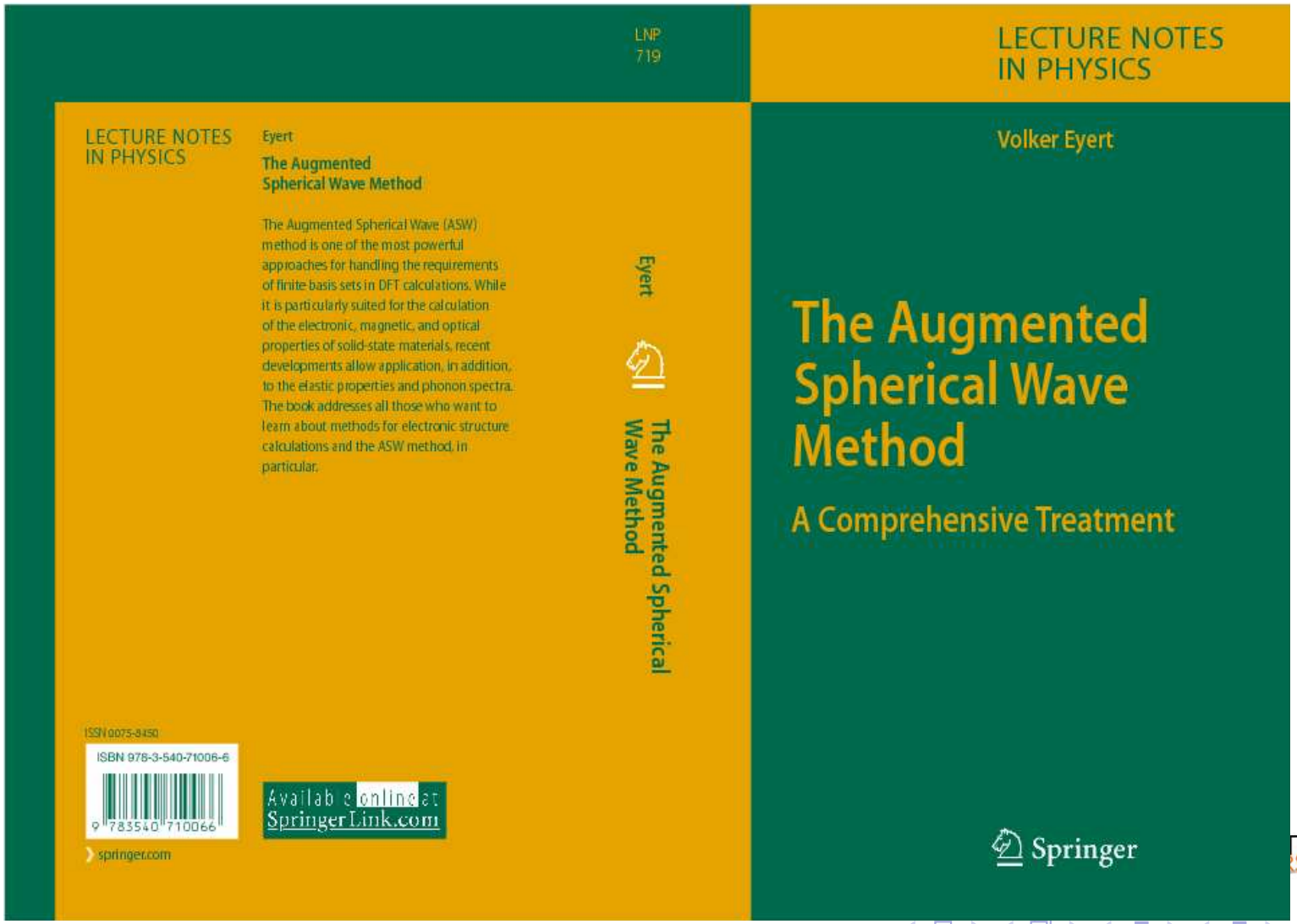
  - different linearization scheme
  - different interstitial energy
  - different implementations

1st Generation (VE, 1990s) IJQC **77**, 1007 (2000)

- completely new, monolithic implementation
- new algorithms $\longrightarrow$ improved accuracy, numerical stability
- much improved functionality, usability, and portability
- all LDA-parametrizations, most GGA-schemes
- many new interpretative tools
- still based on atomic-sphere approximation

ASW Method: Further Reading



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Steps to be Taken

- remove total energy error due to overlap of atomic spheres
  - reintroduce non-overlapping muffin-tin spheres
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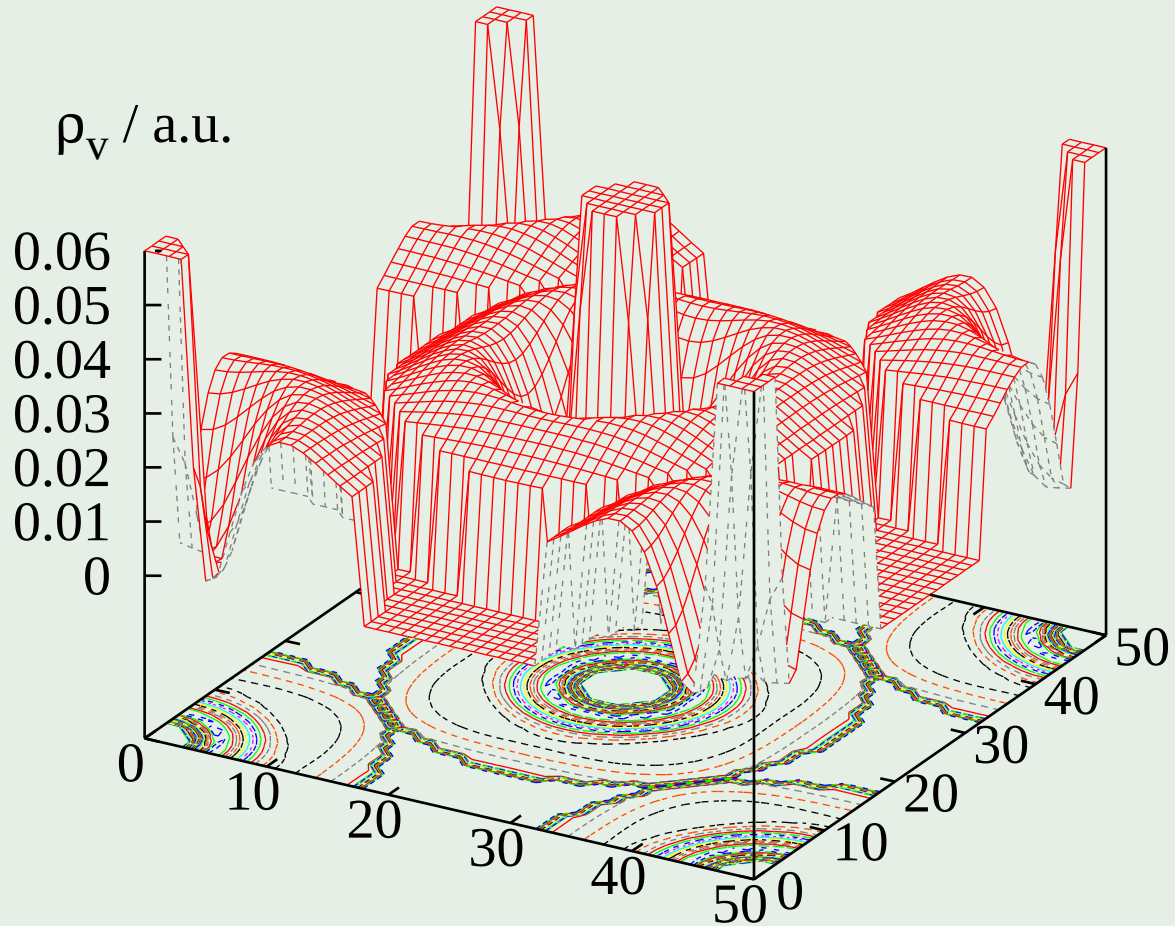
  - inside muffin-tin spheres
    - use spherical-harmonics expansions
  - in the interstitial region
    - no exact spherical-wave representation available!

From Wave Functions to Electron Density

Density inside MT-Spheres (Al)



From Wave Functions to Electron Density

Products of Basis Functions in Interstitial Region

$$p^I(\mathbf{r}) = \sum_n d_n F_n(\mathbf{r})$$

$$\int d^3\mathbf{r}\, F^*_{n'}(\mathbf{r}) p^I(\mathbf{r}) = \sum_n d_n \int d^3\mathbf{r}\, F^*_{n'}(\mathbf{r}) F_n(\mathbf{r})$$

From Wave Functions to Electron Density

Products of Basis Functions in Interstitial Region

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- $F_n(\mathbf{r})$: plane waves
  - integrals exact
  - inefficient
  - Weyrich 1988, Blöchl 1989, VE 1991, Savrasov 1992, Methfessel 2000

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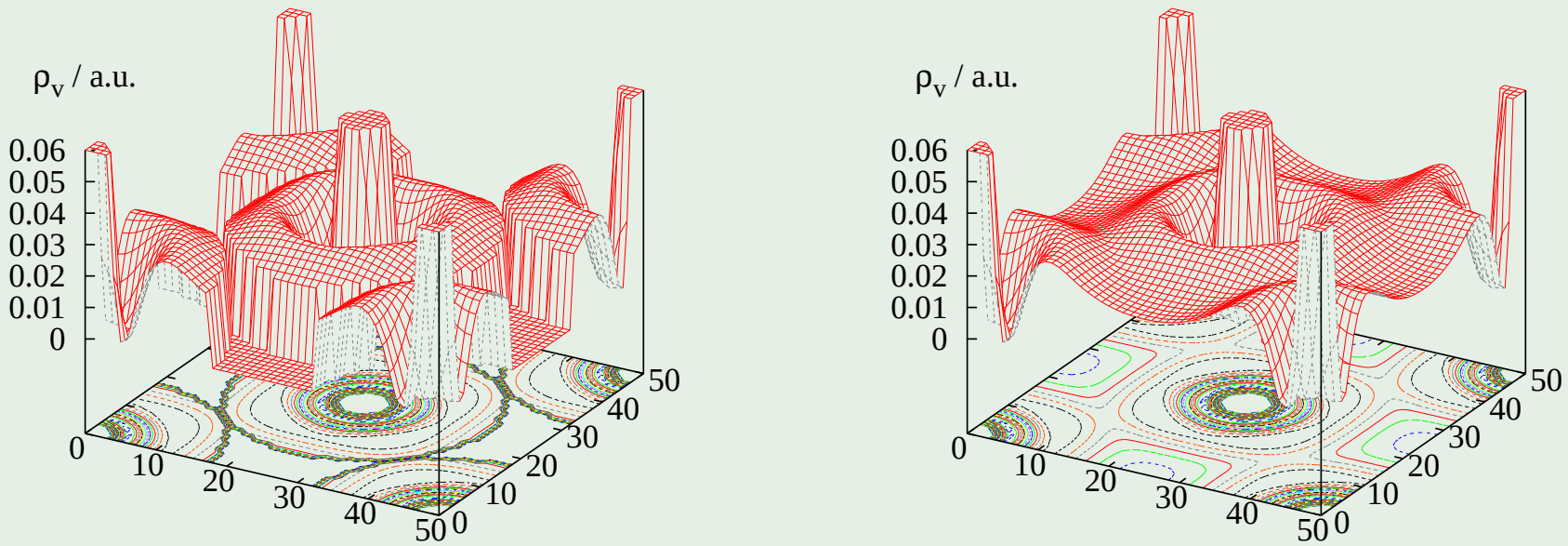
  - Methfessel 1988:
    match values and slopes at MT-sphere surfaces

From Wave Functions to Electron Density

Density from Value/Slope Matching at MT-Radii (Al)



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From Electron Density to Full Potential

Inside Muffin-Tin Spheres

- density, Hartree-potential and xc-potential numerically

Interstitial Region

- density from value/slope matching
- Hartree-potential analytically
- xc-potential from value/slope matching

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From Full Potential to Basis Functions

Previous Approaches

- project full potential to muffin-tin potential
- construct basis functions from muffin-tin potential
- no minimal basis set! (large basis set!)

Present Approach

- project full potential to ASA potential
- construct basis functions from ASA potential
- minimal basis set!

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Comparison of Approaches

Ole K. Andersen

- ASA geometry used for basis functions
  $\rightarrow$ minimal basis set — good!
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Michael S. Methfessel

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Implementation

2nd Generation ASW (VE, 2000s)

- based on 1st generation code
- full-potential ASW method — at $\mathcal{O}$(ASA) speed!
  - electron densities, spin densities
  - electric field gradients
  - elastic properties, phonon spectra
- optical properties
  - based on linear-response theory
  - direct calculation of $\Re\sigma$ and $\Im\sigma$
  - no Kramers-Kronig relations needed
- LDA+U method
  - all „flavours“ for double-counting terms (AMF, FLL, DFT)

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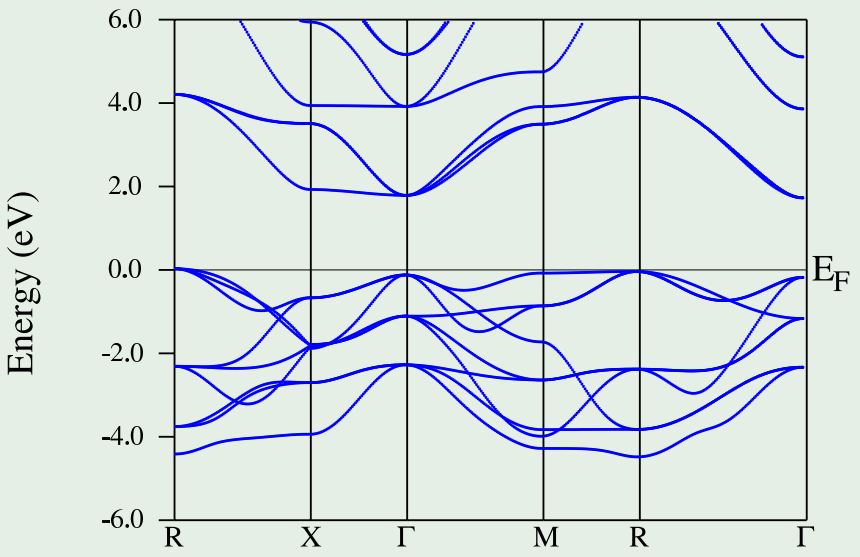
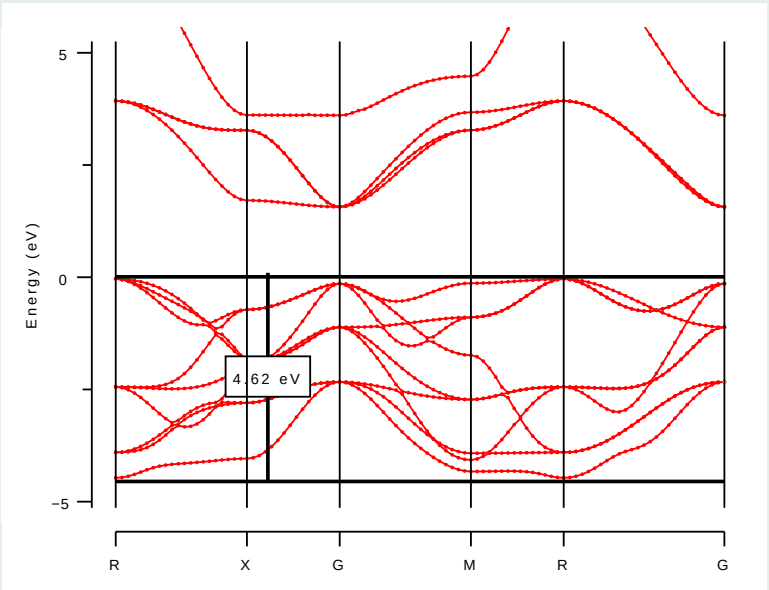
Electronic Structure of $BaTiO_3$

Wien2k



VASP



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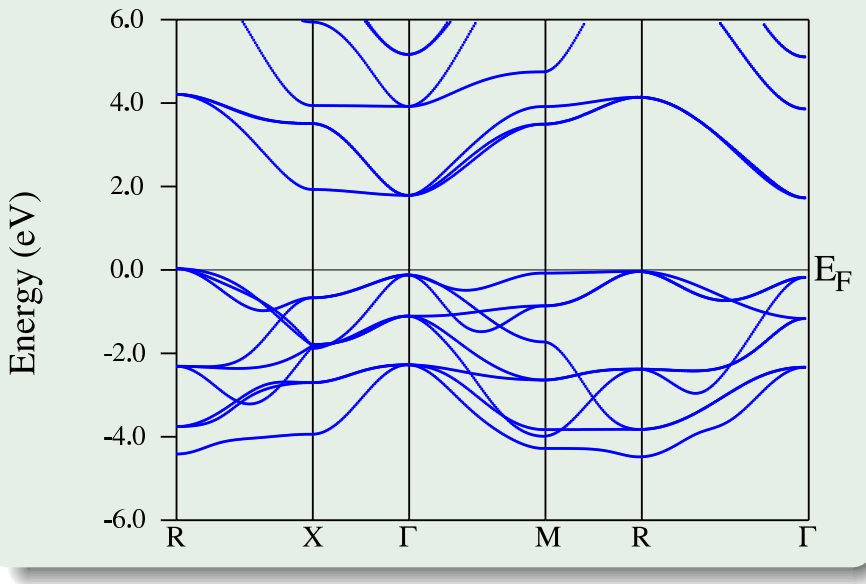
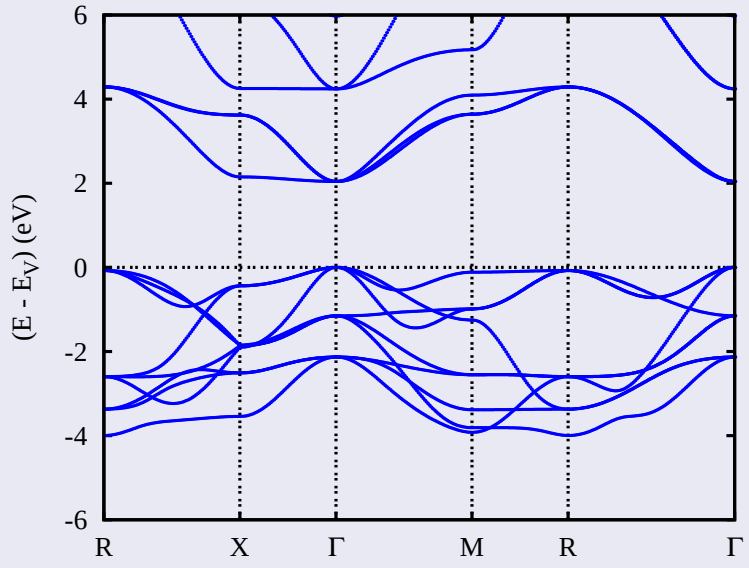


ASW Version 2.2



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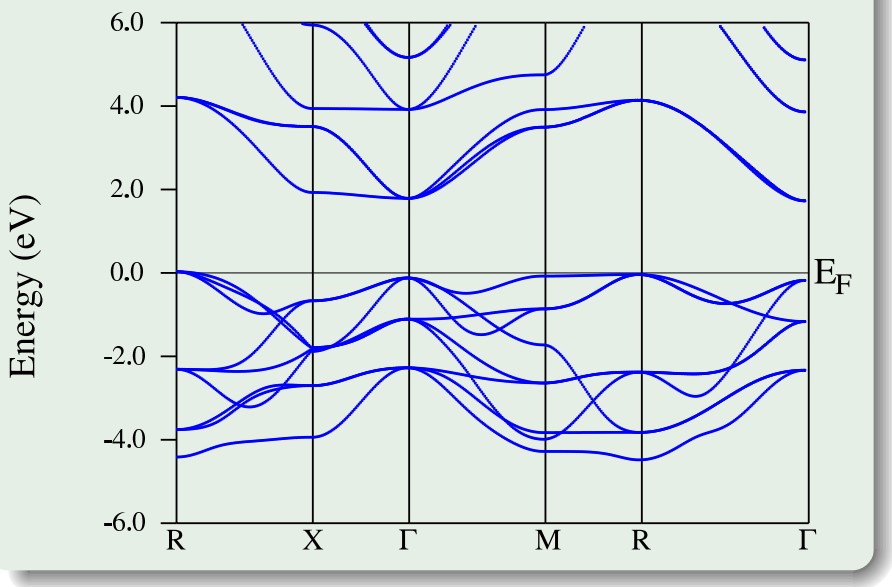
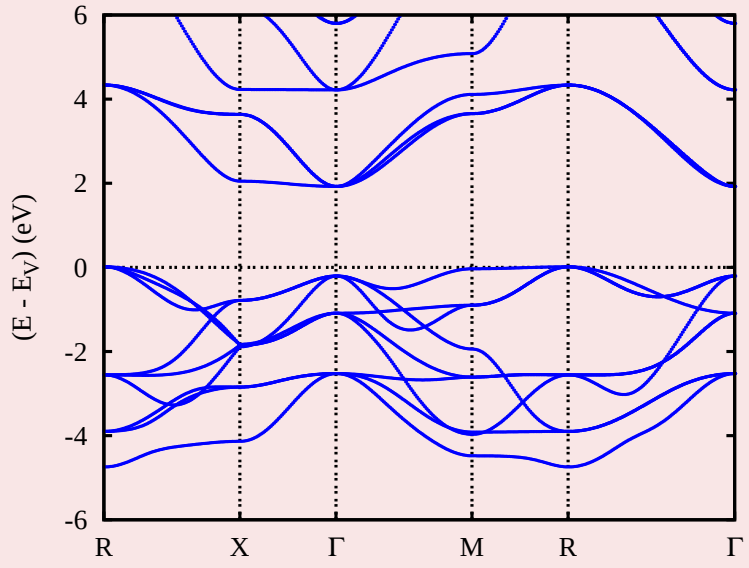


FPASW Version 2.3

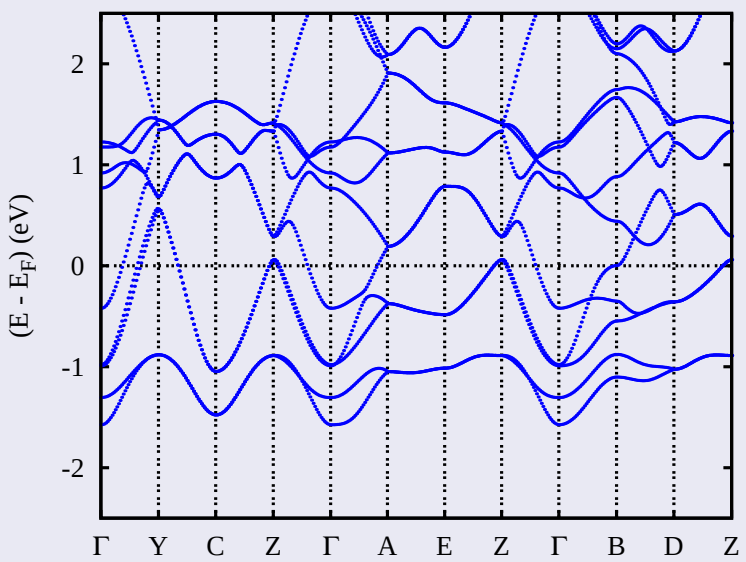


New!

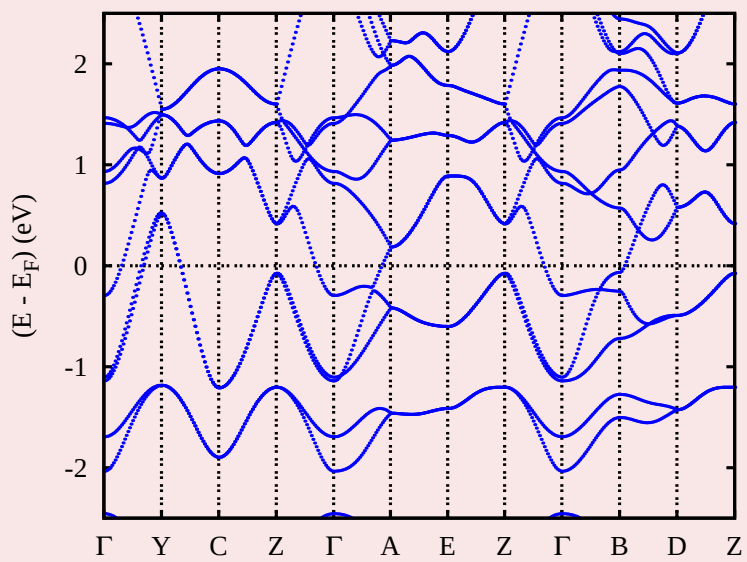
- much better agreement with other full-potential codes (valence-band width, valence states at M-point)

Fermi Surface of MoO_2

ASW Version 1.9



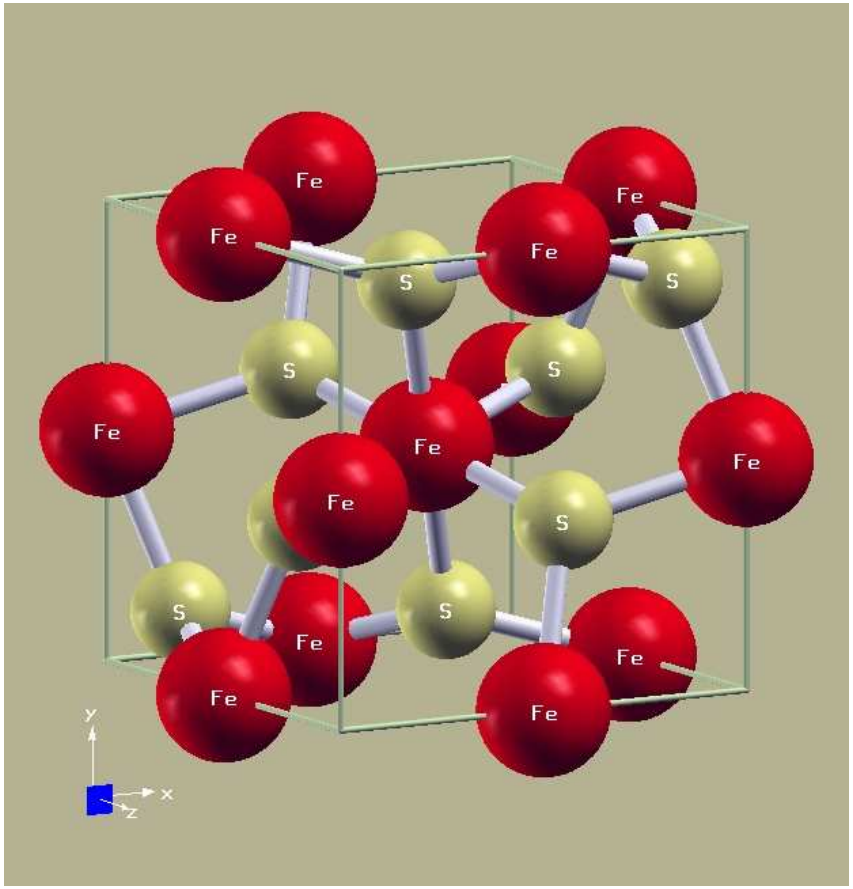
FPASW Version 2.3



New!

- no hole pocket near Z-point
- much better agreement with ARPES, de Haas-van Alphen

Iron Pyrite: FeS_2



Pyrite

- $Pa\bar{3}$ (T_h^6)
- a = 5.4160 Å
- "NaCl structure" sublattices occupied by
  - iron atoms
  - sulfur pairs
- sulfur pairs $\parallel \langle 111 \rangle$ axes
- x_S = 0.38484
- rotated FeS_6 octahedra

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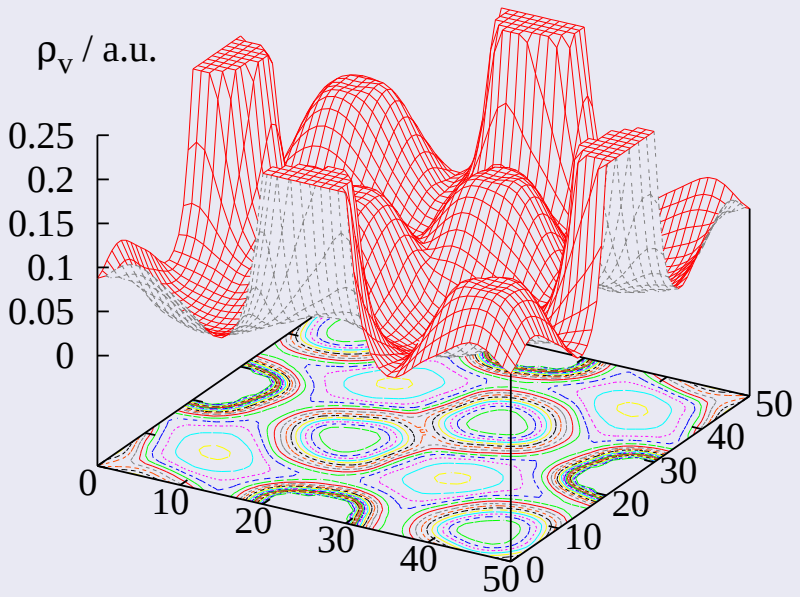
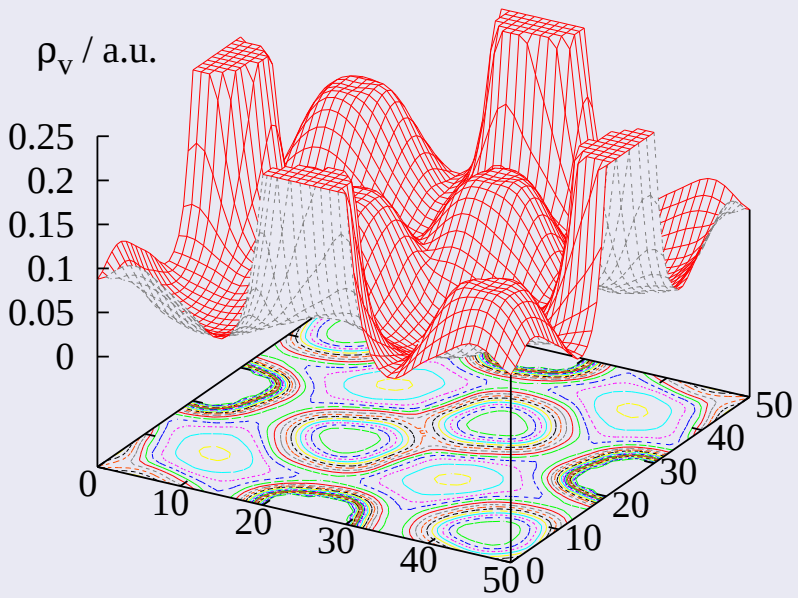
FeS_2: Density and Laplacian

Valence Electron Density

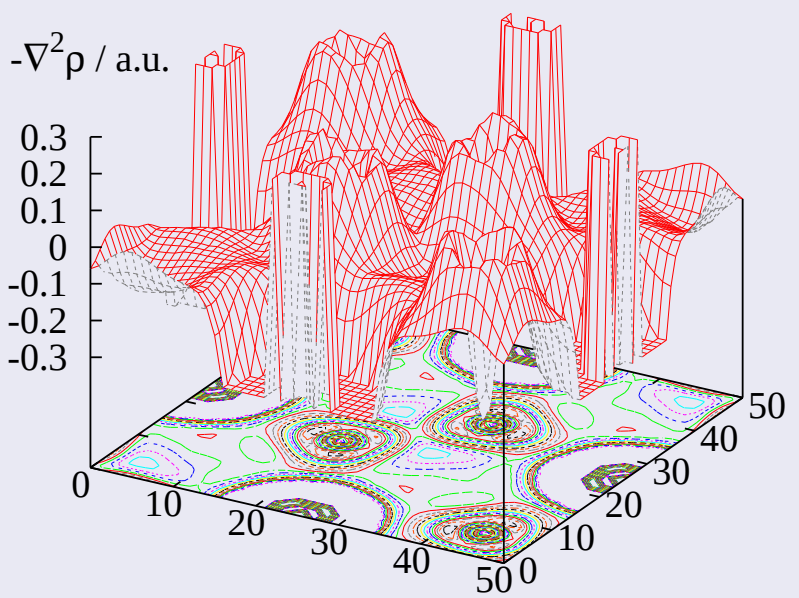


FeS_2: Density and Laplacian

Valence Electron Density



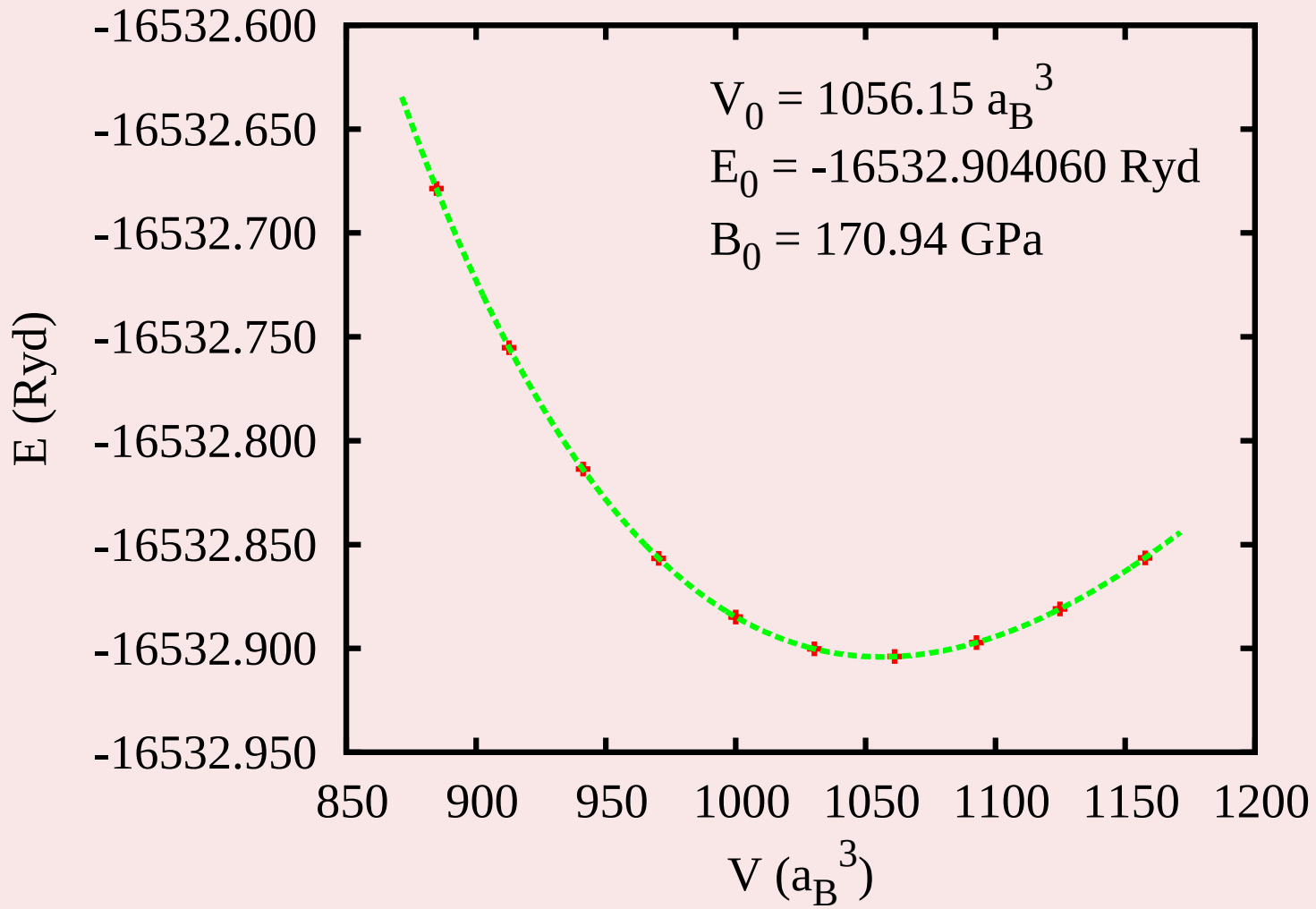
Laplacian of Electron Density



New!

- topological analysis (Bader analysis)

FeS_2: Equilibrium Volume and Bulk Modulus



FeS_2: Equilibrium Volume and Bulk Modulus

Lattice Constant

10.28	NCPP	Zeng and Holzwarth '94
10.02	FPLO	Opahle *et al.* '99
10.17	CRYSTAL98	Muscat *et al.* '02
9.92	CASTEP	Muscat *et al.* '02
10.18	FPASW	present work
10.23	exp.	Finklea *et al.* '76
10.22	exp.	Will *et al.* '84
10.23	exp.	Stevens *et al.* '91

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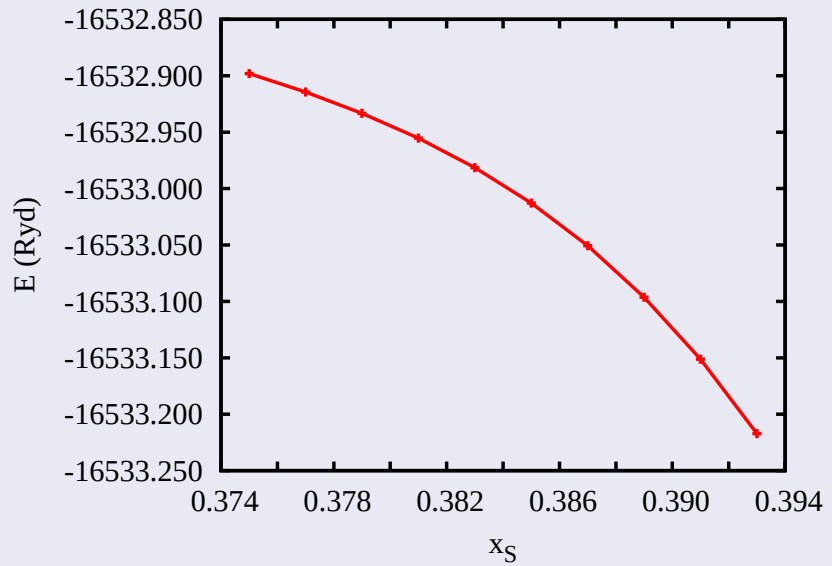
FeS_2: Equilibrium Volume and Bulk Modulus

Bulk Modulus

187	LMTO	Nguyen-Manh *et al.* ’98
185	FPLO	Opahle *et al.* ’99
209	CRYSTAL98	Muscat *et al.* ’02
208	CASTEP	Muscat *et al.* ’02
171	FPASW	present work
148	exp.	Drickamer *et al.* ’66
118	exp.	Will *et al.* ’84
215	exp.	Chattopadhyay and von Schnering ’85
157	exp.	Fujii *et al.* ’86
143	exp.	Jephcoat and Olson ’87
162	exp.	Ahrens and Jeanloz ’87
145	exp.	Blachnik *et al.* ’98

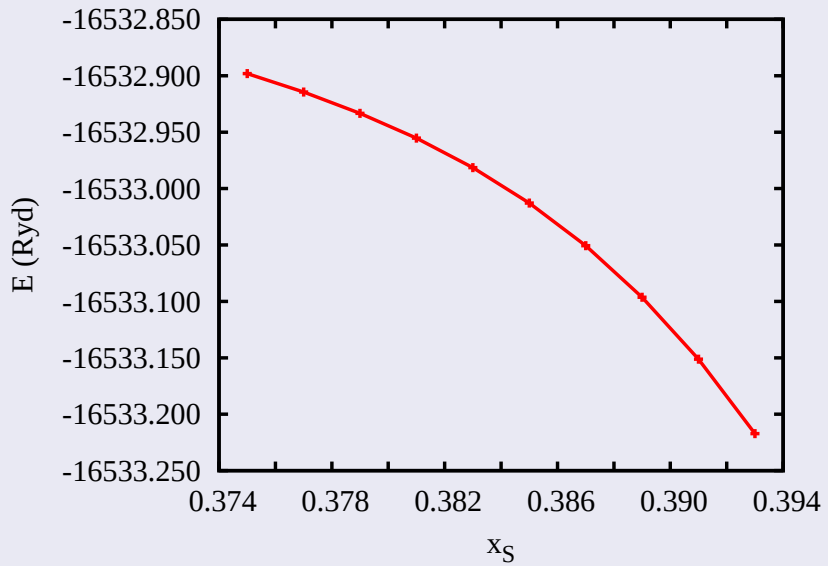
FeS_2: Structure Optimization

ASW Version 2.2

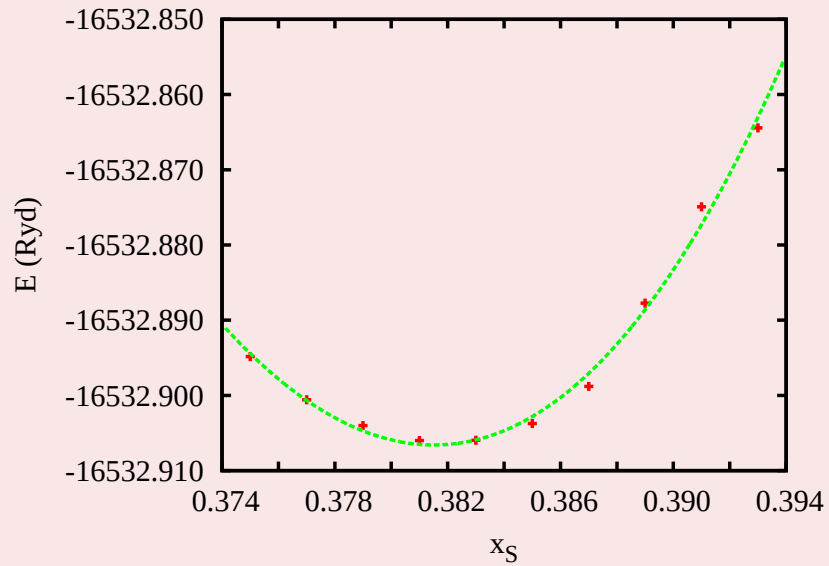


FeS_2: Structure Optimization

ASW Version 2.2



FPASW Version 2.3



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FeS_2: Structure Optimization

Sulfur Position

0.378	NCPP	Zeng and Holzwarth '94
0.377	FPLO	Opahle *et al.* '99
0.378	CRYSTAL98	Muscat *et al.* '02
0.382	CASTEP	Muscat *et al.* '02
0.382	FPASW	present work
0.386	exp.	Finklea *et al.* '76
0.386	exp.	Will *et al.* '84
0.385	exp.	Stevens *et al.* '91

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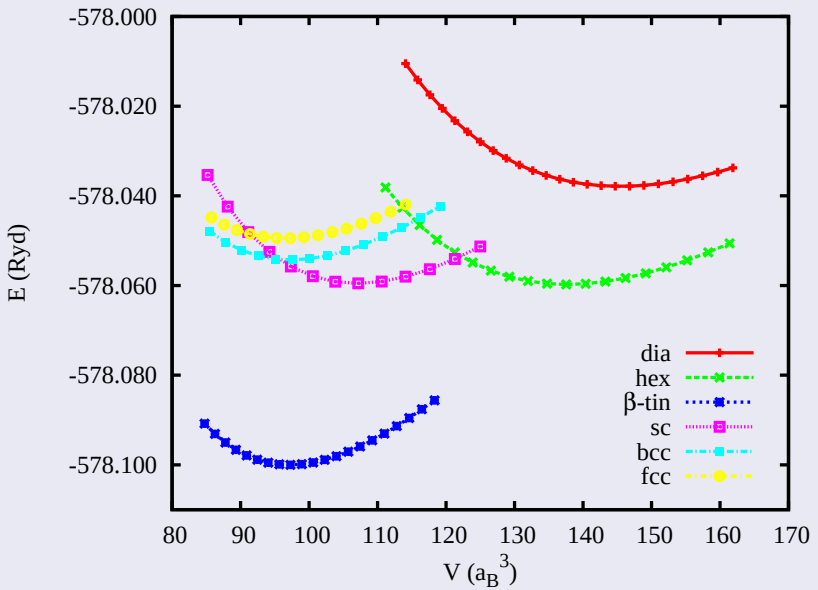
Phase Stability in Silicon

ASW Version 2.2

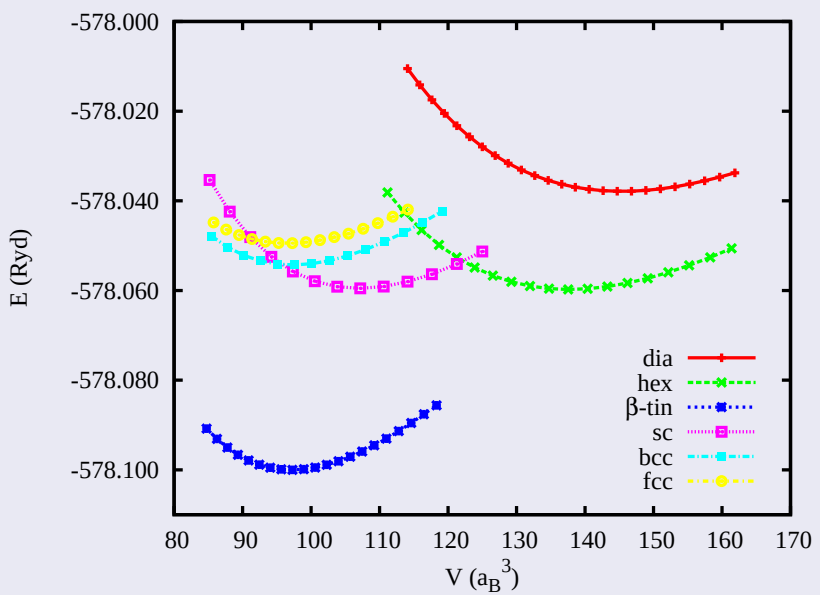


Bad

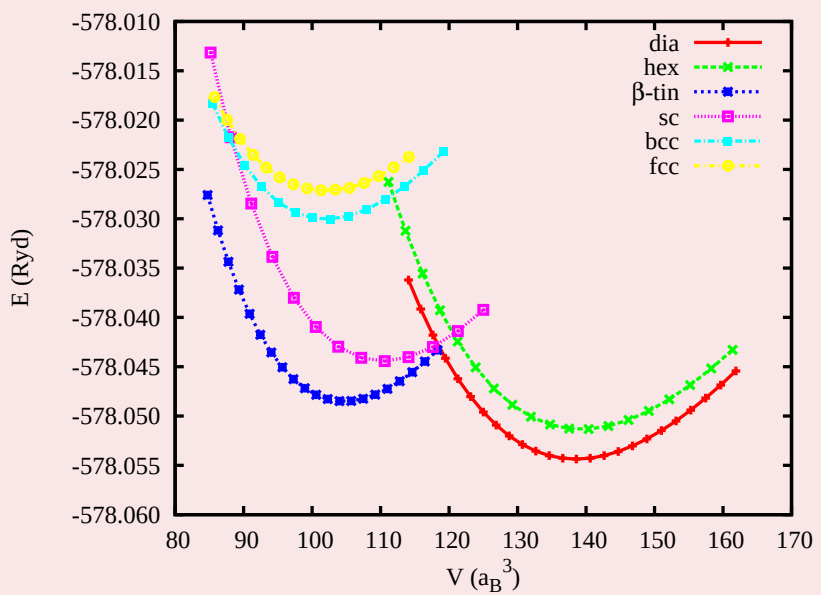
- β-tin structure most stable # nature (diamond structure)

Phase Stability in Silicon

ASW Version 2.2



FPASW Version 2.4

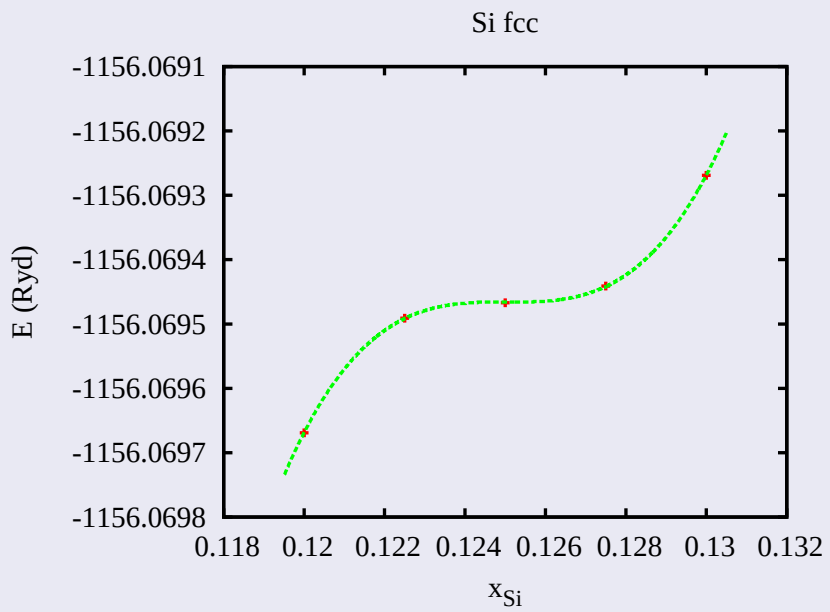


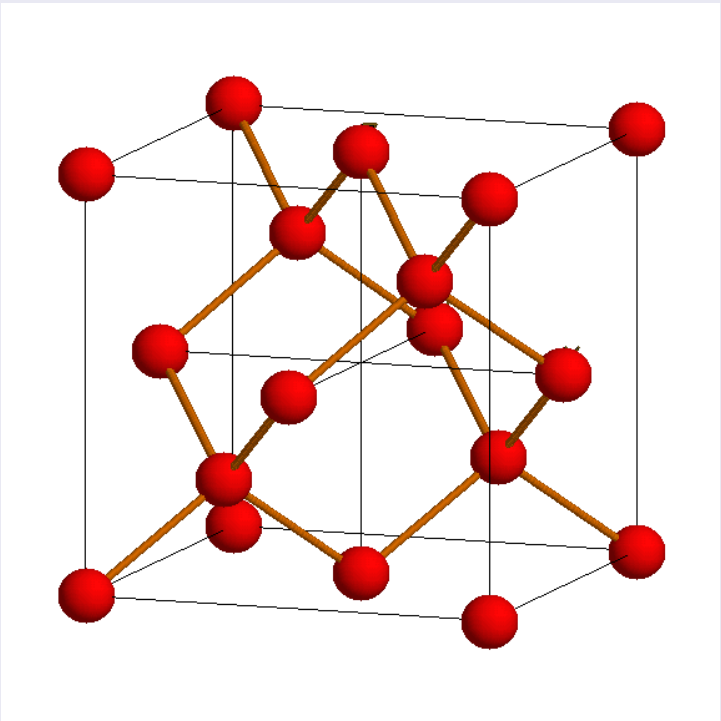
New!

- diamond structure most stable
- pressure induced phase transition to β-tin structure

LTO(Γ)-Phonon in Silicon

ASW Version 2.2



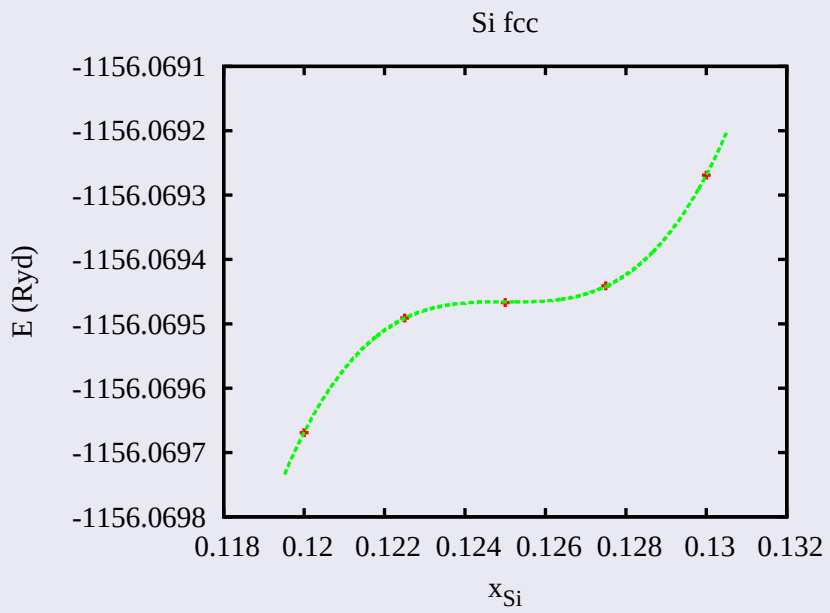


Bad

- no stable Si position # nature

LTO(Γ)-Phonon in Silicon

ASW Version 2.2



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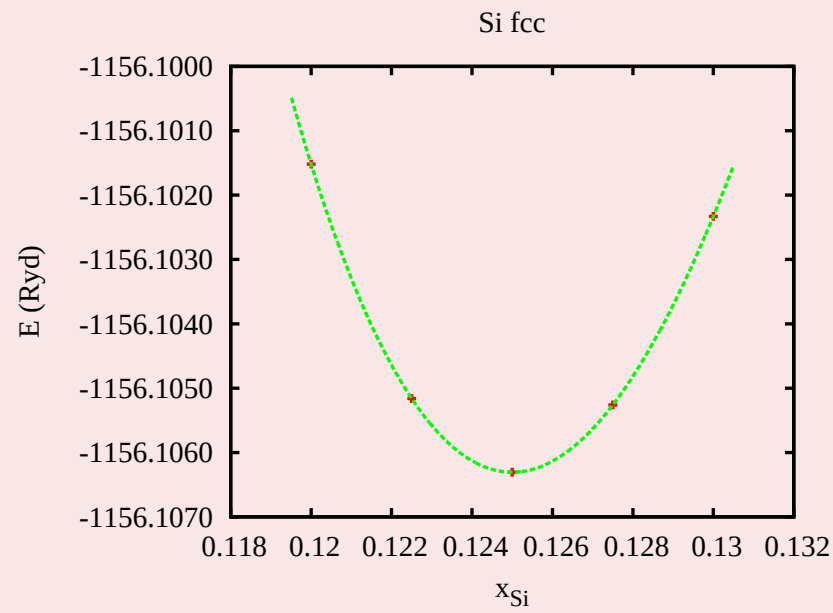


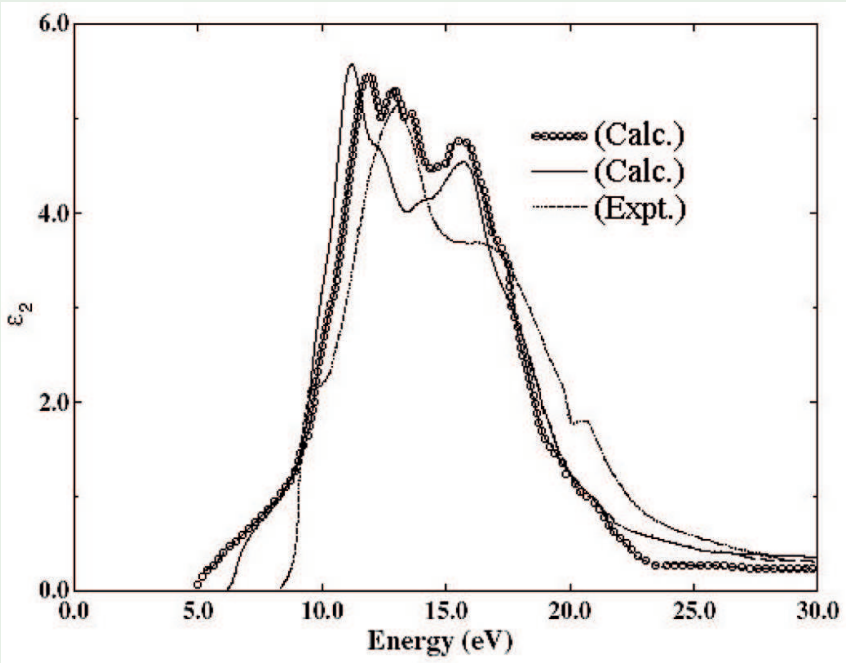
New!

- phonon frequency: $f_{calc} = 15.26\,\text{THz}$ ($f_{exp} = 15.53\,\text{THz}$)

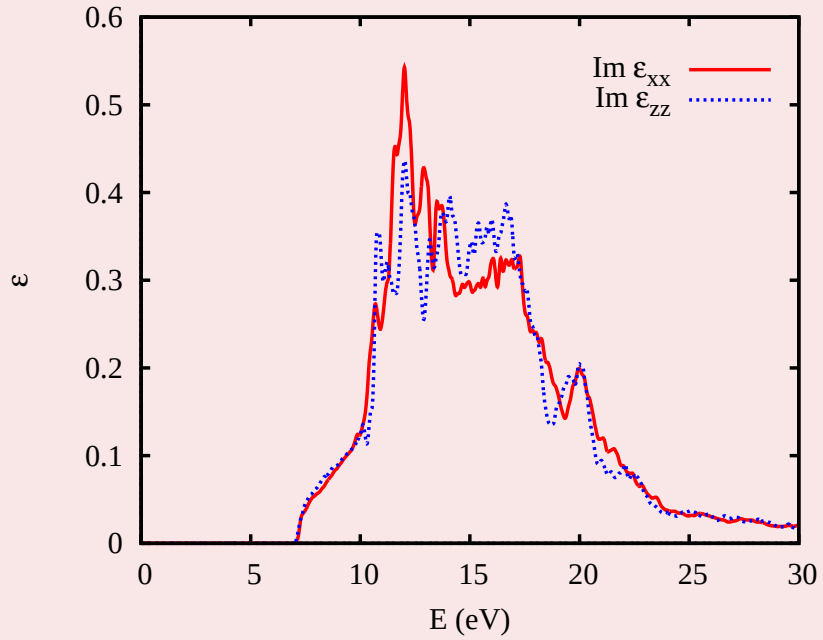
Dielectric Functions of Corundum

Imaginary Part

FLAPW, Hosseini *et al.*, 2005
FPLMTO, Ahuja *et al.*, 2004



FPASW



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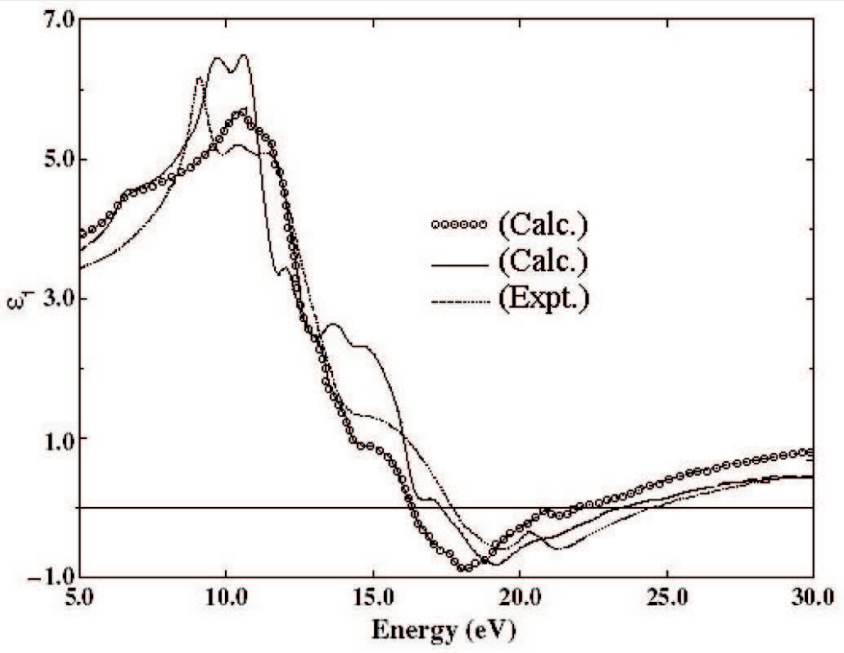
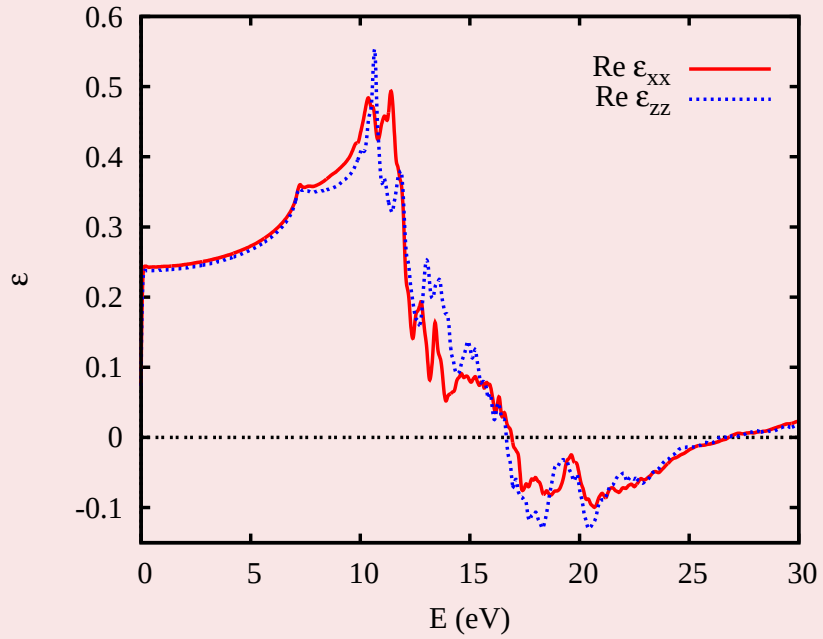
Dielectric Functions of Corundum

Real Part

FLAPW, Hosseini *et al.*, 2005
FPLMTO, Ahuja *et al.*, 2004



FPASW



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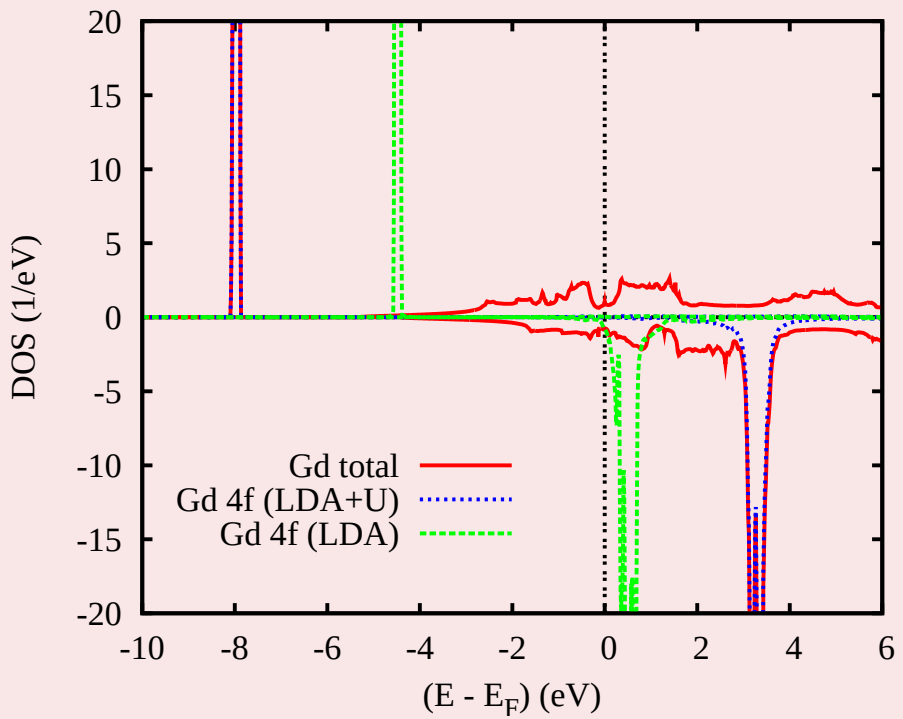
LDA+U-Calculations for Gadolinium

DOS of ferromagnetic Gd



Energetics

	$E_{AF} - E_{FE}$
LDA	-1.601
LDA+U	8.425

(in mRyd/atom)

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Summary

Full-Potential ASW Method (Versions 2.3/2.4)

- ASA Geometry used for Basis Functions
- MT Geometry used for Density and Potential
- Accurate Total Energies
- $\mathcal{O}$(ASA) Speed!
- Optical Properties implemented
- LDA+U-Method implemented

What's Next?

- Forces? Automated Structure Optimization?
- Improved Treatment of Exchange (EXX) and Correlations (LDA+DMFT, EXX+DMFT)?

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Acknowledgments

Darmstadt
SFB 252

Stuttgart
O. K. Andersen

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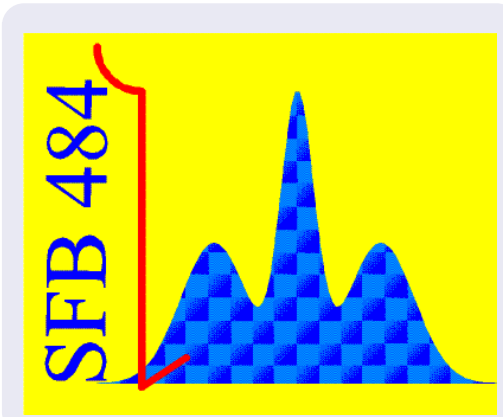
T. Kopp, J. Mannhart,
K.-H. Höck, W. Scherer



Darmstadt
J. Sticht †

Darmstadt
P. C. Schmidt, M. Stephan

Irsee
Thank You for Your Attention!