All-Electron Full-Potential Calculations at $\mathcal{O}$(ASA) Speed

Volker Eyert

Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

Augmented Spherical Wave (ASW) Method

- all-electron method
- based on spherical waves (atomic-like; s, p, d, f)
  - spherical Hankel functions outside augmentation spheres
  - numerical solutions inside augmentation spheres
  - natural interpretation of results
- atomic-sphere approximation (ASA)
  - muffin-tin approximation (MTA), space-filling spheres
  - minimal basis set $\longrightarrow$ very high computational efficiency
  - systematic error in total energy, no 3D-density
- similar to LMTO method (Andersen 1975)

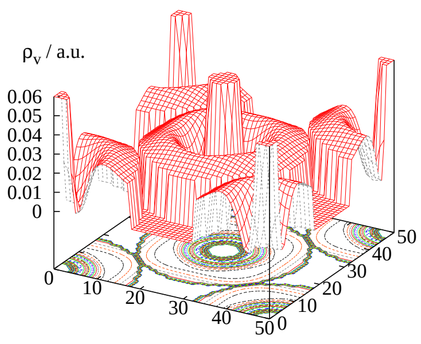
Aim: Full-Potential Spherical-Wave Method

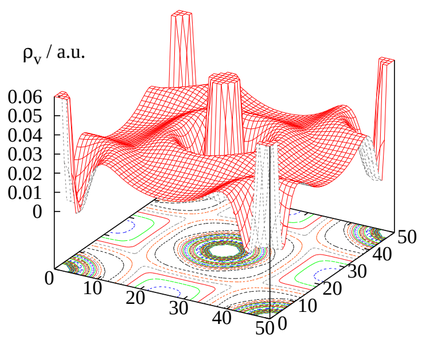
- remove total energy error due to overlap of atomic spheres
  - reintroduce non-overlapping muffin-tin spheres
  - restore interstitial region
- find representation of products of the basis functions

Full-Potential ASW Method

From Wave Function to Electron Density

- spherical-harmonics expansion inside MT-spheres (left figure)
- plus Hankel-function expansion in interstitial region (right figure)
  - coefficients from value/slope-matching at MT-sphere surfaces (Methfessel 1988)





From Electron Density to Full Potential

- MT-spheres: $v_{Hartree}$ and v_{xc} numerically
- interstitial: $v_{Hartree}$ analytically, v_{xc} from value/slope matching

From Full Potential to Basis Functions

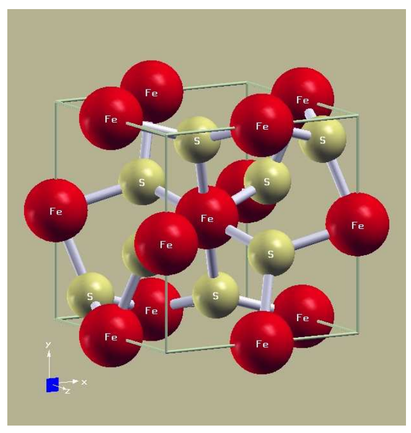
Previous Approaches

- full potential $\longrightarrow$ muffin-tin potential $\longrightarrow$ basis functions
- no minimal basis set! (multiple-κ basis set!)

Present Approach

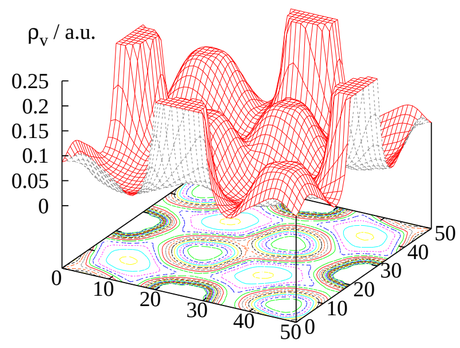
- full potential $\longrightarrow$ ASA potential $\longrightarrow$ basis functions
- minimal basis set!
- computational efficiency maintained $\longrightarrow$ $\mathcal{O}$(ASA) speed!!!

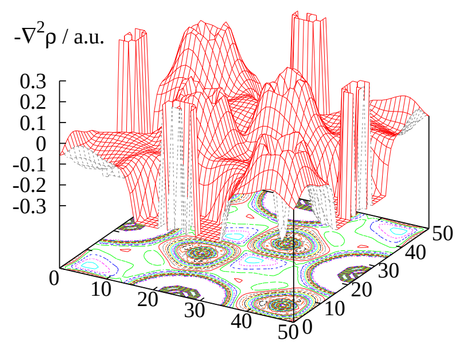
Iron Pyrite: FeS_2



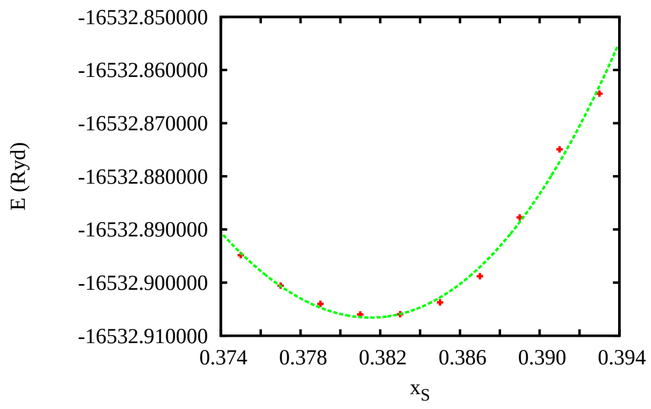
- $Pa\bar{3}$ (T_h^6)
- a = 5.4160 Å
- "NaCl structure" sublattices occupied by
  - iron atoms, sulfur pairs
- sulfur pairs $\parallel \langle 111 \rangle$ axes
- x_S = 0.38484

Density and Laplacian





Structure Optimization



0.378	NCPP
0.377	FPLO
0.378	CRYSTAL98
0.382	CASTEP
0.382	FPASW

Summary

Full-Potential Augmented Spherical-Wave Method

- ASA geometry used for basis functions
  $\longrightarrow$ minimal basis set — good!
- MT geometry used for density and potential
  $\longrightarrow$ accurate total energy — good!
- $\mathcal{O}$(ASA) speed — great!
- electron and spin densities, Laplacians
- elastic properties, phonon spectra
- future: topological analysis, ELF, ELI

Acknowledgments

- W. Scherer, E.-W. Scheidt
- T. Kopp, J. Mannhart
- J. Sticht (†), K.-H. Höck
- P. C. Schmidt, M. Stephan
- DFG: SFB 484, SPP 1178

References