The Augmented Spherical Wave (ASW) Method

Foundation

- Born-Oppenheimer approximation
- density functional theory (DFT)
- local density approximation (LDA) and generalized gradient approximation (GGA) (most parametrizations implemented)

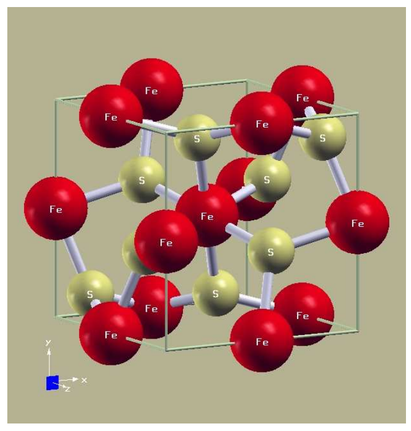
Overview

- all-electron method
  - core electrons fully included
  - full coverage of the periodic table
  - applicable to metals, semiconductors and insulators
- 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
- non-relativistic and scalar-relativistic calculations
- spin-restricted and spin-polarized calculations
- Brillouin-zone integrations based on Monkhorst-Pack mesh
  - simple sampling method
  - high-precision sampling method (Methfessel/Paxton)
  - linear tetrahedron method (including Bl"ochl's correction)
- closed-packed and open crystal structures
  - automated placement of additional interstitial basis functions
  - automated determination of augmentation radii
- efficient convergence acceleration scheme

Properties

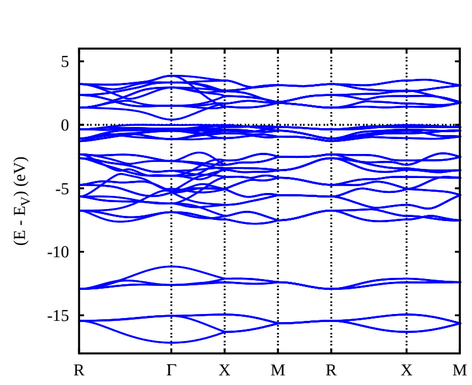
- electronic properties
  - electronic dispersions $\mathrm{E}(\mathbf{k})$ ("band structure")
  - electronic wave functions + projected band structures
  - total/partial (site/state projected) densities of states (DOS)
  - Fermi surfaces
  - optical spectra
  - charge densities at nuclei $\longrightarrow$ isomer shifts
- cohesive properties
  - cohesive energies
  - bulk moduli
- chemical bonding
  - total/partial crystal orbital overlap populations (COOP)
- magnetic properties
  - total and site/state projected magnetic moments
  - magnetic ordering (ferro-, ferri-, antiferromagnetic)
  - magnetic energies
  - spin densities at nuclei $\longrightarrow$ hyperfine fields

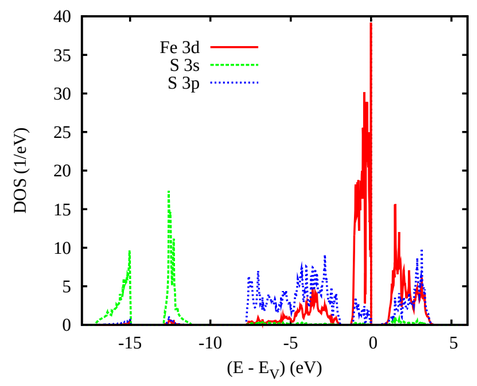
Iron Pyrite: FeS_2



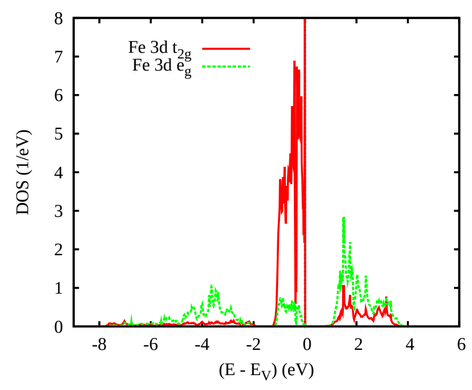
- $Pa\bar{3}$ (T_h^6)
- a = 5.4160 Å
- "NaCl structure" sublattices occupied by
  - iron atoms, sulfur pairs
- sulfur pairs $\parallel \langle 111 \rangle$ axes
- x_S = 0.38484

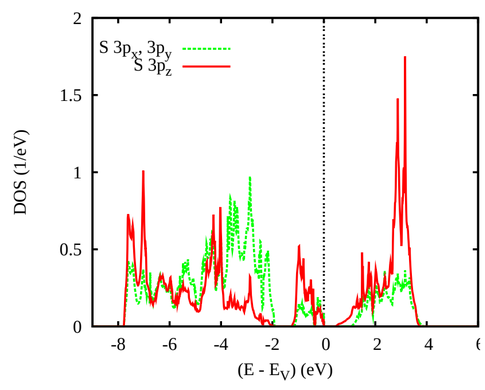
Electronic Bands and Densities of States





Partial Densities of States





References

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