The Augmented Spherical Wave Method

Introduction

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Electronic Structure in a Nutshell

Outline

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ASW?

Meaning: Three Levels of Consciousness

- Augmented Spherical Wave
  (for beginners)

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- Aussersinnliche Wahrnehmung
  (“extrasensory perception”, for the experienced)

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Meaning: Three Levels of Consciousness

- Augmented Spherical Wave
  (for beginners)
- Aussersinnliche Wahrnehmung
  (“extrasensory perception”, for the experienced)
- Always Slightly Wrong
  (for experts)

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Generations

0th Generation, IBM Yorktown Heights, 1970s

- A. R. Williams, J. Kübler, C. D. Gelatt jr.
- original version
- built on the “renormalized atom” concept
- related to O. K. Andersen’s LMTO

0th Generation, Darmstadt, 1980s

- J. Kübler, J. Sticht, V. E., L. Sandratskii
- optimization, vectorization
- non-collinear magnetism
- relativistics, spin-orbit coupling
- full potential code

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- R. A. deGroot, H. van Leuken
- “tight-binding”-like ASW

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- Biosym $\longrightarrow$ MSI $\longrightarrow$ Accelrys
- Electronic Structure Of Crystalline Solids)
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Generations

1st Generation, Europe, 1990s

- new implementation from scratch
- “clean programming”
- new algorithms $\longrightarrow$ accuracy, numerical stability
- improved file handling
- extended flexible basis set
- sphere packing, improved symmetry check
- convergence acceleration schemes
- all LDA-parametrizations, many GGA-schemes
- new interpretative tools

Generations

1st Generation, Angel Fire/Le Mans, 1990s

- Materials Design
- Electronic Structure and Analysis
- commercial version of the 1st generation code

2nd Generation, Europe, 2000s

- linear tetrahedron method
- optical properties
- fast full potential code
- elastic properties, phonon spectra, EFGs

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Features I: The ASW method ...

Foundation

- is based on
  - Born-Oppenheimer approximation
  - density functional theory (DFT)
- uses
  - local density approximation (LDA)
    (all known parametrizations implemented)
  - generalized gradient approximation (GGA)
    (Perdew-Wang 1986, Perdew-Wang 1991, Engel-Vosko 1993, Perdew-Burke-Ernzerhof 1996, Zhang-Yang 1998, Wu-Cohen 2005)
  - exact exchange (future)

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Features II: The ASW method ...

Characteristics

- is an all-electron method
  - core electrons fully relaxed
  - full coverage of periodic table
  - applicable to metal, semiconductors, and insulators
- uses a minimal basis set
  - atomic-like (s, p, d, f) basis functions
  - high computational efficiency
  - intuitive interpretation of results
- allows for
  - non-relativistic and scalar-relativistic calculations
  - spin-restricted and spin-polarized calculations

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Features III: The ASW method ...

Characteristics

- is a linearized method
  - high computational speed
- is fully self-consistent
  - speedup due to efficient convergence acceleration
- performs BZ integrations on Monkhorst-Pack mesh using
  - simple sampling method
  - high-precision sampling method (Methfessel/Paxton)
  - linear tetrahedron method (including Blöchl's correction)
- is suited for closed-packed and open crystal structures
  - automated placement of interstitial basis functions
  - automated determination of augmentation radii

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Electronic

- electronic dispersions $E(\mathbf{k})$ (“band structure”)
- electronic wave functions
  - projected band structures
- total/partial (site/state projected) densities of states (DOS)
- Fermi surfaces
- optical spectra
- electron densities
- electric field gradients
- electron densities at nuclei $\longrightarrow$ isomer shifts
- core level spectra

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Properties II

Cohesive and Elastic

- cohesive energies
- bulk moduli
- elastic constants
- phonon spectra

Chemical

- Laplacians of the electron density
- bonding indicators
  - total/partial crystal orbital overlap populations (COOP)
  - total/partial crystal orbital Hamiltonian populations (COHP)
  - total/partial covalence energies (E_{cov})

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The Code

Programming

- written in Fortran 95
- checked with *ftnchek* and *forcheck*
- 6 main programs for background calculations
- 6 main programs for plotting
- $\approx$ 300 ASW subroutines
- 46 BLAS routines (level 1, 2, 3)
- 77 LAPACK routines
- $\approx$ 110000 lines of source code
  - $\approx$ 25%: BLAS/LAPACK
  - $\approx$ 25%: comments
  - $\approx$ 25%: user guidance
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External Software

Linear Algebra Routine Tasks

... using public-domain standard math. libraries:

- LAPACK - Linear Algebra PACKage
- BLAS - Basic Linear Algebra Subroutines
- ATLAS - Automatically Tuned Linear Algebra Software
- GotoBLAS - K. Goto's fast implementation of the BLAS

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... using public-domain software:

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  - crystal structure
- XCrysDen
  - crystal structure
  - (electron density, Laplacian, ELF, potential)
  - Fermi surface
- Gnuplot
  - (weighted) bands
  - (partial) DOS
  - (partial) COOP, COHP, E_{cov}
  - optical spectra
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Portability

Platforms and Compilers

- IBM
- HP/Compaq
- CRAY/SGI
- SNI
- Sun
- Apple
- PC's running Linux
  - Lahey/Fujitsu f95
  - PGI f90
  - Absoft f95
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Portability

Job Queuing Systems

... accessible by the shell scripts

- IBM's LoadLeveler
- Network Queuing System - NQS
- Portable Batch System - PBS
- Distributed Queuing System - DQS
- Sun Grid Engine - SGE

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Further Reading II


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