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The WIEN2k package is a computer program written in Fortran which performs quantum mechanical calculations on periodic solids. It uses the full-potential (linearized) augmented plane-wave and local-orbitals [FP-(L)APW+lo] basis set to solve the Kohn-Sham equations of density functional theory.

WIEN2k - Wikipedia

Now a new version, WIEN2k, is available, which is based on an alternative basis set. This allows a significant improvement, especially in terms of

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speed, universality, user-friendliness and new features. WIEN2k is written in FORTRAN 90 and requires a UNIX operating system since the programs are linked together via C-shell scripts. It has been implemented successfully on the following computer systems: Pentium systems running under Linux, IBM RS6000, HP , SGI , Compac DEC Alpha, and SUN.

1 Introduction - Carnegie Mellon University

Properties with WIEN2k - III Total energy and forces optimization of internal coordinates, (damped MD, BROYDEN) cell parameter only via E tot(no stress tensor) Phonons via a direct method (based on forces from supercells) interface to PHONON (K.Parlinski) - bands, DOS, thermodynamics, neutrons Pyrochlore structure of Y 2Nb 2O

Introduction to WIEN2k

WIEN2k An Augmented Plane Wave Plus Local Orbitals Program for Calculating

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Crystal Properties User's Guide, WIEN2k
11.1 (Release 11.04.2011) Peter Blaha
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WIEN2k - Carnegie Mellon University

WIEN2k An Augmented Plane Wave +
Local Orbitals Program for Calculating
Crystal Properties revised edition
WIEN2k 08.3 (Release 18/9/2008) Univ.
Prof. Dr. Karlheinz Schwarz Techn.
Universitat Wien" Institut fur
Physikalische und Theoretische Chemie"
Getreidemarkt 9/156 A-1060
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WIEN2k An Augmented Plane Wave Plus
Local Orbitals Program for Calculating
Crystal Properties User's Guide, WIEN2k

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14.2 (Release 10/15/2014) Peter Blaha
Karlheinz Schwarz Georg Madsen Dieter
Kvasnicka Joachim Luitz Vienna
University of Technology Inst. of Physical
and Theoretical Chemistry
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Vienna/Austria

WIEN2k - ALBA (Indico)

Introduction to Solid State theory, DFT
and the APW-method (K.Schwarz)
Introduction to the WIEN2k code
(P.Blaha) This presentation starts out
with an explanation of the basic features
of WIEN2k. discuss the most important
input/output/scf files. Further on details
of tasks like the calculation of DOS and
bandstructures,

Lecture notes from the WIEN2k- workshop 2013 at PennState ...

WIEN2k An Augmented Plane Wave Plus
Local Orbitals Program for Calculating
Crystal Properties User's Guide, WIEN2k
19.1 (Release 06/13/2019) Peter Blaha
Karlheinz Schwarz Georg K. H. Madsen

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Dieter Kvasnicka Joachim Luitz Robert
Laskowski Fabien Tran Laurence D.
Marks Vienna University of Technology
Institute of Materials Chemistry
Getreidemarkt 9/165-TC

WIEN2k

WIEN2k, and the advanced optical response program, Exciting, are the two notable exceptions that include all the electrons in the calculations (called full potential methods).

An introduction to the calculation of valence EELS ...

wien2k¶ WIEN2k performs electronic structure calculations of solids using density functional theory (DFT). It is based on the full-potential (linearized) augmented plane-wave ((L)APW) + local orbitals (lo) method, one of the most accurate schemes for band structure calculations.

WIEN2k - NERSC Documentation

WIEN2k An Augmented Plane Wave Plus

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Local Orbitals Program for Calculating Crystal Properties User's Guide, WIEN2k 16.1 (Release 12/12/2016) Peter Blaha
Karlheinz Schwarz Georg Madsen
Dieter...

WIEN2k -

used as a graphical tool for WIEN2k, a FP-(L)APW program package. The following graphical tasks can be performed by the XCrySDen program:
visualization of crystal structures
graphical selection of k-path inside the Brillouin zone for

XCrySDen - (X-Window) Crystalline Structures and Densities

wien2k_14.2: initialization example / use a graphi - Duration: 6:48. ... Introduction to Project Management | Project Management Basics - Duration: 1:36:42. PMC Lounge Recommended for you.

WIEN2k (Exercise1, outline)

Spin-orbit interaction in Wien2k Wien2k LAPW basis: orbital coordinates - chosen

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in each sphere spin coordinates - global, only z-axis specified by user
Diagonalization of $H+H_{so}$: orbital coord. \equiv spin coord. Wien2k unit cell: Analysis and postprocessing (QTL, wien2wannier) : orbital coord. can be chosen

Spin-orbit physics of iridates with Wien2k

Cubic sodium niobate (NaNbO_3) and tetragonal potassium niobate (KNbO_3) crystals are studied using the Wien2k code.

How study band structure by using wien2k for calculation?

One among the most precise schemes to solve the KS equations is the linearized-augmented-plane-wave (LAPW) method that is employed for example in the computer code WIEN2k to study crystal...

(PDF) DFT calculations of solids with LAPW and WIEN2k

The WIEN2k workshop includes

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elementary and advanced tutorials on DFT, electronic structure calculations, magnetic, optical and spectroscopic properties as well as detailed introduction and hands-on exercises with the WIEN2k program. In addition, there will also be a poster session for presentations by the participants.

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