

PACKAGE ID - 000440MNF00 FEFF 5.03

KWIC TITLE - Ab Initio X-ray Absorption Fine Structure Code

AUTHORS - Zabinsky, S.I.
University of Washington, Seattle, WA (United States)

Rehr, J.J.
University of Washington, Seattle, WA (United States)

Albers, R.C
Los Alamos National Lab., NM (United States)

LIMITATION CODE -COPY **AUDIENCE CODE** - LIM

COMPLETION DATE - 12/07/1992 **PUBLICATION DATE** - 04/27/1992

DESCRIPTION - FEFF5.03 calculates single and multiple-scattering curved wave XAFS spectra, phase shifts and effective scattering amplitudes for cluster of atoms.

PACKAGE CONTENTS - Media Directory; Software Abstract; Media Contains Documentation;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 3.5 diskette

METHOD OF SOLUTION - Code consists of four modules 1) a scattering potential and phase shift code: code uses a relativistic Dirac-Fock-Slater Desclaux atom code within the von Barth-Hedin ground state lda exchange-correlation potential; scattering states are calculated using overlapped atom potentials plus a Hedin-Lundqvist/Quinn complex exchange correlation potential for excited states, referenced to the average interstitial potential; muffin-tin radii are determined automatically from calculated Norman radii; XAFS spectra are referenced to the threshold fermi level, as estimated by electron gas theory; atomic configurations and core-hole lifetimes are built in, and mean free paths are determined from the imaginary part of the average interstitial potential; 2) a path code: code uses heap structure and several importance criteria to explore all significant multiple-scattering paths in order of increasing path length from list of atomic coordinates, and generates a list of single and multiple-scattering paths, paths.dat; 3) a scattering matrix code: code calculates effective scattering matrices used in multiple scattering calculations using the algorithm of Rehr and Albers, and generates feffn.dat files, one for each scattering path; 4) an XAFS code: code ff2chi constructs the XAFS spectrum chi (k) from feff.dat files. Single and multiple scattering Debye-Waller factors are calculated using a correlated Debye model.

COMPUTER - MAINFRAMES

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OPERATING SYSTEMS - Designed to be portable

PROGRAMMING LANGUAGES - FORTRAN 77

SOURCE CODE AVAILABLE (Y/N) - Y

HARDWARE REQS - 2.6 megabytes of memory.

REFERENCES - S.I Zabinsky, J.J. Rehr, and R.C. Albers, FEFF 5 Ab Initio
X-ray Absorption Fine Structure Code, DOE/ER/45415-8, April 27,
1992.

ABSTRACT STATUS - Submitted July 24, 1992.

SUBJECT CLASS CODE - W

KEYWORDS -

COMPUTER PROGRAM DOCUMENTATION
F CODES
SCATTERING AMPLITUDES
PHASE SHIFT
X-RAY DIFFRACTION
FINE STRUCTURE
X RADIATION
ABSORPTION SPECTRA
SOLID CLUSTERS

EDB SUBJECT CATEGORIES -
990200 664200

SPONSOR - DOE/ER

PACKAGE TYPE - AS - IS