

## ATTACHMENT A - DESCRIPTION AND PRICE LIST

### 1. Description

FEFF is an automated code for *ab initio* calculations of XAFS. Several versions of FEFF software are now available: The latest release FEFF8 yields in addition to calculations of XAFS spectra based on the MS path expansion, full multiple scattering calculations of XANES together with a self-consistent calculation of electronic structure, i.e., local densities of states (LDOS) and Fermi energy. FEFF8 also allows for spin-dependent calculations and inclusion of screening effects (core-hole and local field). Like FEFF7, FEFF8 includes relativistic dipole matrix elements and x-ray polarization dependence. Their predecessor FEFF6 only yields semi-relativistic XAFS and XANES, FEFF5 yields only MS XAFS calculations, and FEFF3 yields only single-scattering XAFS calculations. Tabulated XAFS amplitudes and phases based on FEFF3 are also available (FEFF Tables). The FEFF5-8 distributions include an auxiliary code ATOMS, which yields FEFF input files from crystallographic data. Documentation and sample input and output files are also provided.

### 2. Fee for Corporate Use (License, distribution and handling)

New license, distribution and handling fees for corporate clients are as follows: FEFF8 \$2400, FEFF7 \$2100, FEFF6 \$1800, FEFF5 \$1500, and FEFF3 \$900. Fees for each additional system on which the code is installed are 50% of the new license fees. Upgrades (e.g., from FEFF5 to FEFF7) for currently licensed owners of FEFF codes are also 50% of new license fees. See the schedule on the attached price list/order form for details.

### 3. Installation and On-Site Instruction (optional)

An installation fee (\$600 + travel expenses) will provide on-site installation, testing and user instruction.

### 4. Updates and New Releases

All licensees will be informed of major new release availability (anticipated to be about one (1) every two years). Major new releases of FEFF will be available at 50% of the new license fee to licensed users. Updates or bug fixes within a given series (e.g., FEFF6.00 to FEFF6.01) will be provided on request at no charge.

### 5. Payment and Software Delivery

All payments must be payable to the University of Washington by check or money order in US dollars, by electronic bank transfer or credit card, and sent to FEFF Project (please see attached price list for address details). Full payment by check, money order or by credit card is the preferred method of payment and orders which include payment get priority processing. Please mail one copy of the completed license agreement together with the attached order form and your payment. Delivery cannot be made until payment or an official purchase order or a copy of the bank transfer order has been received.

Note: To identify the source of payment, the FEFF invoice number must appear on your payment or bank transfer.

### 6. System Requirements

FEFF software has been designed for portability and should run without modification on most machines. Target machine(s) should have an ANSI standard FORTRAN77 compiler which supports COMPLEX\*16 arithmetic. However, executable versions are also available for n86PCs and 030/040 or Power Macintosh machines. The newest release of FEFF8 typically requires about 512 MB RAM, while previous versions of FEFF8 typically require 64 MB. FEFF7 and earlier typically require 16MB or less.

### 7. Purchasing Details

Please complete the attached order form, including a description of the computer system on which you wish to install the FEFF Software.