Computation of photoelectron and Auger-electron diffraction II. Multiple scattering cluster calculation PAD2

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Abstract

In this paper, we describe the second (PAD2) of the suite of computer programs for the calculation of angle-resolved photo- or Auger-electron diffraction intensities, using a concentric-shell algorithm (CSA). The function of the present program is to evaluate the scattering matrix that relates the wavefunction of an electron immediately after its emission from an atomic core to the wavefield that may be detected outside a sample, using an angular-momentum expansion centered on the emitter atom. This program allows that matrix to be evaluated by any of the following schemes (in ascending order of accuracy, and computer requirements): single scattering (SS), outward multiple scattering (OS) and full multiple scattering (MS). © 1998 Elsevier Science B.V.

PROGRAM SUMMARY

Title of program: PAD2

Catalogue identifier: ADIA

Program Summary URL:
http://www.cpc.cs.qub.ac.uk/cpc/summaries/ADIA

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland

Licensing provisions: none

*Computer for which the program is designed and others on which

it is operable: DEC-alpha and Silicon Graphics workstations, and CRAY and NEC supercomputers

Operating systems under which the program has been tested: UNIX

Programming language used: FORTRAN-77

Memory required to execute with typical data: 8.8 mega-words for test data; could be significantly more for higher electron kinetic energies, or lower symmetry atomic clusters

No. of bits in a word: 64

Has the code been vectorised or parallelized? Partially

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Nature of physical problem
The program PAD2 evaluates the transmission matrix relating the wavefunction of an electron immediately after its emission from an atom to its wavefunction outside a sample, where it may be detected. This matrix is expressed in an angular-momentum basis centered on the emitting atom.

Method of solution
The electron transmission matrix is evaluated by means of an algorithm which first calculates the scattering matrices of a series of concentric shells centered on the emitter. The scattering between the shells is computed by matrix operations on the shell scattering matrices. Both the intra- and inter-shell scattering may be evaluated by taking account of all multiple scattering processes, or by a choice of approximation schemes of increasing accuracy (and of required computer resources).

Restrictions on the complexity of the problem
For photoelectron diffraction, the present codes are restricted to just s, p, d, and f core electrons.

Typical running time
The running time of this program is very dependent on the degree of symmetry of the cluster of atoms centered on the emitter. It is also determined by the size of this cluster and the number of spherical-wave components required to represent the various wave fields computed by the program. For the test data provided, PAD2 took 1 minute and 49 seconds on a Silicon Graphics Indigo^2 computer with an R10000 processor. For other data sets it could take considerably longer.

Unusual features of the program
For correct results, this program should be compiled using the DOUBLE PRECISION option of the compiler.

LONG WRITE-UP

1. Introduction

The history of multiple-scattering calculations for angle-resolved photoemission can be traced at least as far back as the work of Liebsch [1], who treated emission from an adsorbate on a surface. Pendry [2] proposed a theory for angle-resolved valence-band photoemission and Tong and co-workers [3–5] a corresponding treatment for photoemission from molecular orbitals and atomic core states. All these schemes rely on the computational machinery of low energy electron diffraction (LEED) theory for evaluating the multiple electron scattering in ordered atomic layers. The other major class of techniques rely on the short inelastic scattering length of low and medium-energy electrons in solids to restrict the evaluation of the multiple scattering of the photoelectrons to a localized cluster of atoms surrounding the photo-emitter. An advantage of such a technique is the relaxation of the requirement of translational symmetry in the layers of atoms parallel to the surface. Such cluster techniques have been developed by Barton et al. [6,7], Fritzsche [8] and Fadley and co-workers [9]. In such schemes all the inter-atom propagation of the electrons is represented by Green's functions which relate the amplitudes of a spherical-wave expansion of the wave-field about a particular atom to those of the same wave-field about another. The evaluation of these Green functions turns out to be the limiting factor in the speed of such calculations. Therefore fast approximate schemes such as the Taylor-series magnetic quantum number expansion (TS-MQNE) [6], the reduced angular momentum expansion (RAME) [8], and the separable Green's functions of Rehr and Albers [9,10] have been employed to speed up the calculations.

We describe here the application to Auger and photoelectron diffraction, of an *exact* multiple-scattering cluster scheme [11], based on the classification of the cluster into a series of concentric shells, centered on the electron emitter, and containing atoms of approximately the same distance from the emitter. Such a scheme had been earlier proposed for low energy electron diffraction (LEED) by Pendry [12] and implemented by Saldin and Pendry [13]. The idea was to overcome the disastrous N^3 scaling of computer time of traditional layer methods, where N is the number of atoms per two-dimensional unit cell in each layer.

2. Multiple-scattering theory

When an atom emits an electron by an Auger or photoemission process, the resulting wave-field could be written as the following linear combination, with amplitudes $B_L^{(0)}$, of outgoing spherical waves:

$$\sum_L B_L^{(0)} h_l^{(1)}(kr) Y_L(\hat{\boldsymbol{r}}) , \tag{1}$$

where $(lm) \equiv L$ are angular momentum quantum numbers, $\boldsymbol{r}$ is a position vector with respect to an origin at the emitter, k the wave-number of the emitted electrons, $h_l^{(1)}$ a Hankel function of order l and Y_L a spherical harmonic. (Note that, in this paper, the generic amplitude $B_L^{(0)}$ represents either the quantity $B_{nL_c,L}^{(0)}$, as defined in paper I [17], for photoemission, or the amplitude $B_{\text{Aug},L}^{(0)}$ for Auger emission). The extent of the propagation of the wave (1) through a material will depend on the fairly short inelastic scattering length, and hence be restricted to a localized cluster of atoms surrounding the emitter. For computational convenience we divide the cluster into a series of N concentric shells centered on the emitter. We also suppose that the total electron wave-field between the qth and the $(q+1)$th shells takes the same form as (1), but with expansion coefficients $B_L^{(q)}$, which we collectively represent by the vector $\boldsymbol{B}^{(q)}$. Thus the task of determining the electron wave-field emerging to some external detector after multiple scattering with all atoms of the cluster is effectively one of evaluating the vector $\boldsymbol{B}^{(N)}$, representing the corresponding expansion coefficients of the wave-field propagating outwards from the Nth shell.

The elements of the vector $\boldsymbol{B}^{(N)}$ may be computed from known values of $\boldsymbol{B}^{(0)}$ by the following algorithm [12,13]:

$$\boldsymbol{B}^{(N)} = \boldsymbol{B}^{(0)} \mathbf{S}^{(N)} , \tag{2}$$

where the matrix $\mathbf{S}^{(N)}$ may be evaluated by the following pair of coupled recursion relations:

$$\mathbf{S}^{(q+1)} = \mathbf{S}^{(q)} (\mathbf{I} - \mathbf{T}_{q+1}^{\text{OI}} \mathbf{J}_q^{\text{IO}})^{-1} (\mathbf{I} + \mathbf{T}_{q+1}^{\text{OO}}) \tag{3}$$

and

$$\mathbf{J}_{q+1}^{\text{IO}} = \mathbf{T}_{q+1}^{\text{IO}} + (\mathbf{I} + \mathbf{T}_{q+1}^{II}) \mathbf{J}_q^{\text{IO}} (\mathbf{I} - \mathbf{T}_{q+1}^{\text{OI}} \mathbf{J}_q^{\text{IO}})^{-1} (\mathbf{I} + \mathbf{T}_{q+1}^{\text{OO}}) , \tag{4}$$

with the starting conditions

$$\mathbf{S}^{(0)} = \mathbf{I} \tag{5}$$

and

$$\mathbf{J}_0^{\text{IO}} = \mathbf{t}_c , \tag{6}$$

where $\mathbf{t}_c$ is the t-matrix of the emitter atom.

In the above expressions, $\mathbf{I}$ is a unit matrix, and the elements of the scattering matrices T_q^{OO}, T_q^{OI}, T_q^{II} and T_q^{IO} of the qth shell are given by

$$T_{qLL'}^{\text{OO}} = \sum_{iL_i} \sum_{jL_j} g_{LL_i}^{oi} T_{L_iL_j}^{ij} \tilde{g}_{L_jL'}^{jo} , \tag{7}$$

$$T_{qLL'}^{\text{OI}} = \sum_{iL_i} \sum_{jL_j} g_{LL_i}^{oi} T_{L_iL_j}^{ij} g_{L_jL'}^{jo} , \tag{8}$$

$$T_{qLL'}^{II} = \sum_{iL_i} \sum_{jL_j} \tilde{g}_{LL_i}^{oi} T_{L_iL_j}^{ij} g_{L_jL'}^{jo} , \tag{9}$$

and

$$T_{qLL'}^{\mathrm{IO}} = \sum_{iL_i} \sum_{jL_j} \tilde{g}_{LL_i}^{oi} T_{L_iL_j}^{ij} \tilde{g}_{L_jL'}^{jo} , \tag{10}$$

where

$$g_{LL'}^{ij} = 4\pi(1 - \delta_{ij}) \sum_{l''m''} i^{l-l'-l''}(-1)^{m'+m''} h_{l''}^{(1)}(k|\boldsymbol{r}_j - \boldsymbol{r}_i|) Y_{l''-m''}(\boldsymbol{r}_j \stackrel{\frown}{} \boldsymbol{r}_i) \int Y_{lm} Y_{l''m''} Y_{l'-m'} \, d\Omega \tag{11}$$

is a propagator from atom i of position vector $\boldsymbol{r}_i$ to atom j of position vector $\boldsymbol{r}_j$ in the qth shell. $\tilde{g}_{LL'}^{ij}$ is the same as $g_{LL'}^{ij}$ except that $j_{l''}$ is substituted for $h_{l''}^{(1)}$. The superscript o in the propagators represents the central emitter atom.

The intra-shell multiple scattering is represented by the elements $T_{L_iL_j}^{ij}$ of the matrix [14,15]

$$\mathbf{T} = \mathbf{H}^{-1} , \tag{12}$$

where

$$H_{L_iL_j}^{ij} = t_{L_i}^{(i)-1} \delta_{ij} \delta_{L_iL_j} - g_{L_iL_j}^{ij} \tag{13}$$

are the elements of the real-space Korringa–Kohn–Rostocker (KKR) matrix $\mathbf{H}$ and $t_{L_i}^{(i)}$ is an element of the (diagonal) t-matrix of atom i.

3. The outward scattering approximation

At medium electron kinetic energies, where atomic scattering factors tend to be forward peaked, the "outward" multiple-scattering approximation may enable angle-resolved diffraction intensities to be calculated to reasonable accuracy. This takes advantage of the unique geometry of the concentric shells, yields calculated diffraction patterns practically indistinguishable from those from a full multiple-scattering calculation, affords about an order of magnitude speed-up of the computations, and requires much less computer memory.

The approximation is based on the fact that when a medium-energy electron is incident upon an atom, it is most likely to suffer only *small*-angle scattering, as is now well attested to by numerous publications, e.g. [16]. It is possible to exploit this near-forward scattering behavior in the CSA in two ways: (1) by the neglect of intra-shell multiple scattering, and (2) by the successive transmission approximation to inter-shell multiple scattering. The successive transmission approximation assumes that an outward traveling spherical wave incident on an atomic shell has a negligible backward scattered (i.e., inward traveling) component.

Intra-shell multiple scattering can be turned off by neglecting the intra-shell propagators $g_{L_iL_j}^{ij}$ in (13) above. This is equivalent to making the approximation

$$T_{L_iL_j}^{ij} \approx t_{L_i}^{(i)} \delta_{ij} \delta_{L_iL_j}. \tag{14}$$

in Eqs. (7)–(10).

The inclusion of only forward propagation during the inter-shell multiple scattering is accomplished by setting the *out–in* scattering matrices, $\mathbf{T}_q^{\mathrm{OI}}$, equal to zero. Then the scattering matrix of the entire cluster takes on the particularly simple form,

$$\mathbf{S}^{(N)} \simeq (\mathbf{I} + \mathbf{T}_0^{\mathrm{OO}})(\mathbf{I} + \mathbf{T}_1^{\mathrm{OO}}) \cdots (\mathbf{I} + \mathbf{T}_N^{\mathrm{OO}}) . \tag{15}$$

Note that both these simplifications, which together we term the outward-scattering approximation, avoid the matrix inversion operations necessary for the evaluation of full multiple scattering (see Eqs. (3), (4),

and (12) above), thus substantially reducing computer-time requirements. Nevertheless, the outward-scattering approximation includes all single-scattering events and all significant multiple-scattering pathways, particularly those which do not contain scattering angles greater than about 90°.

4. Overview of PAD programs

To simulate angle-revolved electron diffraction with the PAD programs, it is necessary to run PAD1, PAD2, and PAD3 in sequence as shown in the flow chart on Fig. 1 of paper I of this series. The sequence is important since the compilation of PAD2 and PAD3 may be performed correctly only after PAD1 is executed. This is due to the fact that the INCLUDE file generated by PAD1 is used to determine the sizes of arrays used by PAD2 and PAD3 during their executions. In summary, PAD1 generates a concentric-shell cluster and control parameters, PAD2 calculates the cluster transmission matrix $\mathbf{S}^{(N)}$, and PAD3 uses this matrix and other information specified in the original input file "pad-inpt.dat" to simulate electron diffraction patterns from different types of PD experiments.

5. Program structure of PAD2

The main program of PAD2 calls the subroutine PHASE to read the phase shifts at room temperature on unit 5 for each atom species and then calls CLUSYM, which is the main controlling routine of the program.

CLUSYM calls CLREAD to read `cluster.out` from FORTRAN unit 4. That data set contains the information for setting up the concentric-shell cluster. CLUSYM determines the symmetry of the cluster from the data read in from `cluster.out` and then calls the SHLSYM routine, which returns the shell scattering matrices, T, in a symmetrized single center expansion about the emitter atom.

SHLSYM calculates the scattering matrices, $\mathbf{T}$, of the specified shell of atoms surrounding the emitter, including all intra-shell multiple scattering. This is done by assembling and inverting the symmetry-folded Korringa–Kohn–Rostocker (KKR) matrix, $\mathbf{H}$. That matrix is assembled using the symmetrized propagators supplied by the subroutine GSYM to calculate the shell transmission and reflection matrices $\mathbf{T}^{OI}$, $\mathbf{T}^{II}$, $\mathbf{T}^{IO}$, and $\mathbf{T}^{OO}$.

If the input data specifies no intra-shell multiple scattering, the subroutine SINGLE is called in place of SHLSYM to compute the shell $\mathbf{T}$ matrices.

CLUSYM calls the routine OSFB1 to evaluate the "out–in" reflection matrix (expanded about the emitter atom) of a pair of adjacent shells, the outer one of which is characterized by the out–in reflection matrix, and the inner one by the full set of its scattering matrices $\mathbf{T}$.

Inside a loop over shells, CLUSYM calls TOTMAT if a full inter-shell multiple scattering (MS) calculation is requested, or it calls TOTMUL if the outward-scattering (OS) approximation to inter-shell multiple scattering is chosen, or else it calls TOTSGL if inter-shell multiple scattering is neglected altogether, as in the single-scattering (SS) approximation.

6. Input and output

The input and include files of PAD2 are those generated by PAD1. PAD2 outputs a cluster scattering matrix, `tot.dat`, on unit 9, for input to the third program of this series (PAD3).

It should be noted that when the outward scattering (OS) approximation is used, a special version of PAD2, named PAD2OS, which requires much less computer memory, may be used to replace PAD2. This program may be obtained directly from the authors.

7. Test run

The test run calculates core-level O-1*s* PD, for an electron kinetic energy of 60 eV, for experiment type of PD3, illustrated in Fig. 1c of paper III [18] of this set of papers. The O atom is assumed to occupy a 4-fold hollow site on a Ni(001) surface. In this run the full multiple-scattering option (IFWD=0) is chosen. Only a part of the output file is shown, because it is rather lengthy.

Acknowledgements

References

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TEST RUN INPUT

```
cluster.out: Output file from pad1.f (stream 5)
             Input file to pad2.f (stream 4)
             Input file to pad3.f (stream 4)
MULTIPLE SCATTERING CALCULATION FOR PD AND AD

   2    1    6    6    0    4   28    0
  13    0    0        NO.  1 N=  5 R= 2.6
  18    0    0        NO.  2 N= 12 R= 4.0
  21    0    0        NO.  3 N= 12 R= 5.0
  24    0    0        NO.  4 N= 16 R= 5.9
  27    0    0        NO.  5 N= 21 R= 6.6
  28    0    0        NO.  6 N=  4 R= 6.8
 1.84  -0.369   3.67
   4    1    1    0.0000    0.0000    0.0000
   5    2                                              NO. 1
   2    4   2.00000   2.35177   2.35177   1.54958   3.669   1.9   45
   2    4   2.00000  -2.35177   2.35177   1.54958   3.669   1.9  135
   2    4   2.00000  -2.35177  -2.35177   1.54958   3.669   1.9  225
   2    4   2.00000   2.35177  -2.35177   1.54958   3.669   1.9  315
   2    1   1.00000   0.00000   0.00000   4.87550   4.875   2.6    0
  12    3                                              NO. 2
   2    4   2.00000   4.70353   0.00000   4.87550   6.774   3.6    0
   2    4   2.00000   0.00000   4.70353   4.87550   6.774   3.6   90
   2    4   2.00000  -4.70353   0.00000   4.87550   6.774   3.6  180
   2    4   2.00000   0.00000  -4.70353   4.87550   6.774   3.6  270
   2    4   2.00000   7.05530   2.35177   1.54958   7.597   4.0   18
   2    4   2.00000  -2.35177   7.05530   1.54958   7.597   4.0  108
   2    4   2.00000  -7.05530  -2.35177   1.54958   7.597   4.0  199
   2    4   2.00000   2.35177  -7.05530   1.54958   7.597   4.0  289
   2    4   2.00000   2.35177   7.05530   1.54958   7.597   4.0   71
   2    4   2.00000  -7.05530   2.35177   1.54958   7.597   4.0  161
   2    4   2.00000  -2.35177  -7.05530   1.54958   7.597   4.0  252
   2    4   2.00000   7.05530  -2.35177   1.54958   7.597   4.0  342
  12    3                                              NO. 3
   2    4   2.00000   4.70353   4.70353   4.87550   8.247   4.4   45
   2    4   2.00000  -4.70353   4.70353   4.87550   8.247   4.4  135
   2    4   2.00000  -4.70353  -4.70353   4.87550   8.247   4.4  225
   2    4   2.00000   4.70353  -4.70353   4.87550   8.247   4.4  315
   2    4   2.00000   2.35177   2.35177   8.20141   8.850   4.7   45
   2    4   2.00000  -2.35177   2.35177   8.20141   8.850   4.7  135
   2    4   2.00000  -2.35177  -2.35177   8.20141   8.850   4.7  225
   2    4   2.00000   2.35177  -2.35177   8.20141   8.850   4.7  315
   1    4   2.00000   9.40706   0.00000   0.00000   9.407   5.0    0
   1    4   2.00000   0.00000   9.40706   0.00000   9.407   5.0   90
   1    4   2.00000  -9.40706   0.00000   0.00000   9.407   5.0  180
   1    4   2.00000   0.00000  -9.40706   0.00000   9.407   5.0  270
  16    4                                              NO. 4
   2    4   2.00000   7.05530   7.05530   1.54958  10.097   5.3   45
   2    4   2.00000  -7.05530   7.05530   1.54958  10.097   5.3  135
   2    4   2.00000  -7.05530  -7.05530   1.54958  10.097   5.3  225
   2    4   2.00000   7.05530  -7.05530   1.54958  10.097   5.3  315
   2    4   2.00000   9.40706   0.00000   4.87550  10.595   5.6    0
   2    4   2.00000   0.00000   9.40706   4.87550  10.595   5.6   90
   2    4   2.00000  -9.40706   0.00000   4.87550  10.595   5.6  180
```

```
    2    4    2.00000    0.00000  -9.40706    4.87550  10.595   5.6  270
    2    4    2.00000    7.05530   2.35177    8.20141  11.071   5.9   18
    2    4    2.00000   -2.35177   7.05530    8.20141  11.071   5.9  108
    2    4    2.00000   -7.05530  -2.35177    8.20141  11.071   5.9  199
    2    4    2.00000    2.35177  -7.05530    8.20141  11.071   5.9  289
    2    4    2.00000    2.35177   7.05530    8.20141  11.071   5.9   71
    2    4    2.00000   -7.05530   2.35177    8.20141  11.071   5.9  161
    2    4    2.00000   -2.35177  -7.05530    8.20141  11.071   5.9  252
    2    4    2.00000    7.05530  -2.35177    8.20141  11.071   5.9  342
   21    6                                                          NO. 5
    2    1    1.00000    0.00000   0.00000   11.52733  11.527   6.1    0
    2    4    2.00000    9.40706   4.70353    4.87550  11.593   6.1   26
    2    4    2.00000   -4.70353   9.40706    4.87550  11.593   6.1  116
    2    4    2.00000   -9.40706  -4.70353    4.87550  11.593   6.1  207
    2    4    2.00000    4.70353  -9.40706    4.87550  11.593   6.1  297
    2    4    2.00000    4.70353   9.40706    4.87550  11.593   6.1   63
    2    4    2.00000   -9.40706   4.70353    4.87550  11.593   6.1  153
    2    4    2.00000   -4.70353  -9.40706    4.87550  11.593   6.1  244
    2    4    2.00000    9.40706  -4.70353    4.87550  11.593   6.1  334
    2    4    2.00000   11.75883   2.35177    1.54958  12.091   6.4   11
    2    4    2.00000   -2.35177  11.75883    1.54958  12.091   6.4  101
    2    4    2.00000  -11.75883  -2.35177    1.54958  12.091   6.4  192
    2    4    2.00000    2.35177 -11.75883    1.54958  12.091   6.4  282
    2    4    2.00000    2.35177  11.75883    1.54958  12.091   6.4   78
    2    4    2.00000  -11.75883   2.35177    1.54958  12.091   6.4  168
    2    4    2.00000   -2.35177 -11.75883    1.54958  12.091   6.4  259
    2    4    2.00000   11.75883  -2.35177    1.54958  12.091   6.4  349
    2    4    2.00000    4.70353   0.00000   11.52733  12.450   6.6    0
    2    4    2.00000    0.00000   4.70353   11.52733  12.450   6.6   90
    2    4    2.00000   -4.70353   0.00000   11.52733  12.450   6.6  180
    2    4    2.00000    0.00000  -4.70353   11.52733  12.450   6.6  270
    4    1                                                          NO. 6
    2    4    2.00000    7.05530   7.05530    8.20141  12.916   6.8   45
    2    4    2.00000   -7.05530   7.05530    8.20141  12.916   6.8  135
    2    4    2.00000   -7.05530  -7.05530    8.20141  12.916   6.8  225
    2    4    2.00000    7.05530  -7.05530    8.20141  12.916   6.8  315
EMITTED ELECTRONS IN STATES OF L= 1
B_(Aug,lm)^((O)) AMPLITUDES FOR AD
0.000E+00 0.958E-01 0.958E-01 0.958E-01
NO. OF lm_c STATES, NO. OF lm STATES:
        1                 3
B_(L,nL_c)^(0)', l, m, VALUES FOR PD
( 0.00, 0.00)  1 -1
( 1.00, 0.00)  1  0
( 0.00, 0.00)  1  1
   45.0    0.0       X-RAY POLARIZATION VECTOR, THETA AND PHI
NUMBER OF SPECIES IN THE CLUSTER            2
 1 ATOM(S) OF SPECIES 1, 16 ATOM(S) OF SPECIES 2,
TRANSLATIONAL VECTOR   A(X,Y)=
(4.978000000000000,0.0000000000000000E+00) (ANGSTROMS)
             AND   B(X,Y)=
(0.0000000000000000E+00,4.978000000000000) (ANGSTROMS)
ATOM POSITIONS IN UNIT CELL
  0.250   0.250   0.820 OF SPECIES 1 ATOM 1
  0.000   0.000   0.000 OF SPECIES 2 ATOM 1
  0.500   0.000   0.000 OF SPECIES 2 ATOM 2
  0.000   0.500   0.000 OF SPECIES 2 ATOM 3
```

```
   0.500    0.500    0.000 OF SPECIES 2 ATOM 4
   0.250    0.250   -1.760 OF SPECIES 2 ATOM 5
   0.250    0.750   -1.760 OF SPECIES 2 ATOM 6
   0.750    0.250   -1.760 OF SPECIES 2 ATOM 7
   0.750    0.750   -1.760 OF SPECIES 2 ATOM 8
   0.000    0.000   -3.520 OF SPECIES 2 ATOM 9
   0.500    0.000   -3.520 OF SPECIES 2 ATOM10
   0.000    0.500   -3.520 OF SPECIES 2 ATOM11
   0.500    0.500   -3.520 OF SPECIES 2 ATOM12
   0.250    0.250   -5.280 OF SPECIES 2 ATOM13
   0.250    0.750   -5.280 OF SPECIES 2 ATOM14
   0.750    0.250   -5.280 OF SPECIES 2 ATOM15
   0.750    0.750   -5.280 OF SPECIES 2 ATOM16
NOTE! X&Y IN FRACTIONAL COORDINATES.
POLAR ANGLE  FROM            0 TO          90
WITH A STEP OF           1
AZIMUTHAL ANGLE FROM         0 TO        360
WITH A STEP OF           1
ELECTRON KINETIC ENERGY       50.00000000000000     (eV)
INNER-POTENTIAL              -10.00000000000000     (eV)
BINDING ENERGY          -536.0000000000000    (eV)
MAXIMUM CLUSTER RADIUS        7.000000000000000    (ANGSTROMS)
SURFACE CUT-OFF POINT         1.058000000000000    (ANGSTROMS)
NUMBER OF PHASE SHIFTS               4
DEBYE TEMPERATURE
999.00 K FOR SPECIES 1, 450.00 K FOR SPECIES 2,
ATOMIC MASS
 16.00 MOLE FOR SPECIES 1,  58.70 MOLE FOR SPECIES 2,
NO MIRROR SYMMETRY IN THE CLUSTER!!!
MAX. ANGUL. MOMENT. QUANT. #, LOUT          28
NUMBER OF ATOMS IN THE CLUSTER              71
SHORTEST DISTANCE BETWEEN ATOMS     1.941638612100614
ELECTRON MEAN-FREE-PATH IS CHOSEN FROM UNIVERSAL CURVE
============================ END ========================
```

TEST RUN OUTPUT

`tot.dat` follows: Output file from `pad2.f` (stream 9)
              Input file to `pad3.f` (stream 6)

```
1    1 ( 0.782E+00, 0.859E-01)
1    3 (-0.565E-01,-0.148E+00)
1    7 (-0.427E-01, 0.402E-01)
1   13 (-0.139E-01,-0.772E-01)
1   17 ( 0.387E-01, 0.156E-01)
1   21 (-0.109E-01,-0.762E-02)
1   25 ( 0.387E-01, 0.156E-01)
1   27 ( 0.937E-01, 0.242E-02)
1   31 (-0.955E-01,-0.623E-01)
1   35 ( 0.937E-01, 0.242E-02)
1   39 ( 0.513E-01, 0.135E-01)
1   43 (-0.362E-01,-0.752E-02)
1   47 ( 0.513E-01, 0.135E-01)
1   53 ( 0.291E-01,-0.213E-02)
1   57 ( 0.171E-02, 0.104E-02)
1   61 ( 0.291E-01,-0.213E-02)
1   65 ( 0.765E-02, 0.273E-01)
1   69 ( 0.192E-01, 0.684E-01)
1   73 ( 0.478E-01, 0.258E-01)
1   77 ( 0.192E-01, 0.684E-01)
1   81 ( 0.765E-02, 0.273E-01)
1   83 ( 0.217E-01, 0.179E-01)
1   87 (-0.529E-02, 0.129E-01)
1   91 (-0.127E-01, 0.351E-01)
1   95 (-0.529E-02, 0.129E-01)
1   99 ( 0.217E-01, 0.179E-01)
1  103 ( 0.115E-01, 0.184E-01)
1  107 ( 0.407E-01,-0.843E-02)
1  111 (-0.130E-01, 0.287E-01)
1  115 ( 0.407E-01,-0.843E-02)
1  119 ( 0.115E-01, 0.184E-01)
1  125 (-0.179E-01,-0.434E-01)
1  129 ( 0.394E-01, 0.219E-01)
1  133 (-0.929E-02, 0.526E-01)
1  137 ( 0.394E-01, 0.219E-01)
1  141 (-0.179E-01,-0.434E-01)
1  145 (-0.674E-02,-0.322E-02)
1  149 (-0.836E-02,-0.453E-01)
1  153 ( 0.238E-01, 0.154E-01)
1  157 (-0.926E-02, 0.423E-01)
1  161 ( 0.238E-01, 0.154E-01)
1  165 (-0.836E-02,-0.453E-01)
1  169 (-0.674E-02,-0.322E-02)
1  171 (-0.166E-01, 0.275E-01)
1  175 (-0.336E-01,-0.718E-02)
1  179 (-0.974E-02,-0.128E-01)
1  183 (-0.219E-01, 0.718E-02)
1  187 (-0.974E-02,-0.128E-01)
1  191 (-0.336E-01,-0.718E-02)
1  195 (-0.166E-01, 0.275E-01)
1  199 (-0.302E-01,-0.411E-02)
1  203 ( 0.659E-03,-0.373E-01)
```

```
1  207 (-0.149E-01,-0.559E-01)
1  211 (-0.697E-02,-0.304E-01)
1  215 (-0.149E-01,-0.559E-01)
1  219 ( 0.659E-03,-0.373E-01)
1  223 (-0.302E-01,-0.411E-02)
1  229 (-0.222E-01,-0.108E-01)
1  233 ( 0.315E-01, 0.291E-02)
1  237 (-0.368E-02,-0.267E-01)
1  241 ( 0.155E-01, 0.609E-02)
1  245 (-0.368E-02,-0.267E-01)
1  249 ( 0.315E-01, 0.291E-02)
1  253 (-0.222E-01,-0.108E-01)
1  257 (-0.256E-01, 0.274E-01)
1  261 (-0.151E-01, 0.129E-01)
1  265 (-0.196E-01, 0.203E-01)
1  269 (-0.696E-02,-0.890E-02)
1  273 ( 0.830E-04, 0.103E-01)
1  277 (-0.696E-02,-0.890E-02)
1  281 (-0.196E-01, 0.203E-01)
1  285 (-0.151E-01, 0.129E-01)
1  289 (-0.256E-01, 0.274E-01)
1  291 (-0.185E-01,-0.185E-01)
1  295 (-0.992E-02, 0.195E-01)
1  299 (-0.111E-01,-0.261E-01)
1  303 ( 0.148E-01,-0.115E-01)
1  307 ( 0.218E-01,-0.380E-01)
1  311 ( 0.148E-01,-0.115E-01)
1  315 (-0.111E-01,-0.261E-01)
1  319 (-0.992E-02, 0.195E-01)
1  323 (-0.185E-01,-0.185E-01)
1  327 ( 0.188E-01,-0.114E-01)
1  331 (-0.108E-01, 0.160E-01)
1  335 ( 0.282E-01,-0.109E-01)
1  339 ( 0.119E-01, 0.922E-02)
1  343 ( 0.425E-01,-0.216E-01)
1  347 ( 0.119E-01, 0.922E-02)
1  351 ( 0.282E-01,-0.109E-01)
1  355 (-0.108E-01, 0.160E-01)
1  359 ( 0.188E-01,-0.114E-01)
1  365 ( 0.140E-01, 0.102E-02)
1  369 (-0.157E-01, 0.310E-02)
1  373 ( 0.103E-01, 0.211E-01)
1  377 (-0.778E-02, 0.237E-02)
1  381 ( 0.230E-01, 0.218E-02)
1  385 (-0.778E-02, 0.237E-02)
1  389 ( 0.103E-01, 0.211E-01)
1  393 (-0.157E-01, 0.310E-02)
1  397 ( 0.140E-01, 0.102E-02)
1  401 ( 0.320E-03,-0.204E-01)
1  405 ( 0.492E-02,-0.147E-01)
1  409 (-0.814E-02, 0.503E-03)
1  413 (-0.101E-02, 0.111E-01)
1  417 (-0.275E-02,-0.749E-02)
```