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"Silicon Band Structure Calculation"

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The program BANDS1 is a FORTRAN 77 code that calculates the bandstructure of a face centered cubic semiconductor, using the local pseudopotential method.

The input provided in the code are for silicon. In particular:

```
C-----------------------------------------------------------------------
C                                                                 INPUTS
C-----------------------------------------------------------------------
C     Inputs (Silicon considered here):
C
C     CONSTA = Lattice constant (in Angstroms)
C     NBASIS = Atoms in the basis (here diamond lattice)
C     NSITES = Number of sites included in the calculation
C     PSEUDi = Pseudopotential Fourier components
C     EMAX   = Maximum energy (cutoff)
C     NEIGEN = Number of eigenvalue branches considered
C     NSTEP  = Number of step in momentum
C     STEPK  = Mesh size in momentum space
C-----------------------------------------------------------------------
      CONSTA =  5.43097D0
      NBASIS =  2
      NSITES =  16
      PSEUD1 = -0.224D0
      PSEUD2 =  0.055D0
      PSEUD3 =  0.072D0
      EMAX   =  10.D0
      NEIGEN =  10
      NSTEP  =  10
      STEP   =  0.005
```

Once the code is run, the results for the band structure are placed in two files, `VBAND.OUT` and `CBAND.OUT`, for valence band (4 branches) and conduction band (6 branches), respectively.

The code constructs the Direct Lattice basis vectors of the primitive cell, using the following variables

```
C-----------------------------------------------------------------------
C                                                          DIRECT LATTICE
C-----------------------------------------------------------------------
C     BASIS(i,j) = basis vectors of primitive cell
C                  (face centered cubic lattice)
C                  i  = 1,2,3  vector index
C                  j  = 1,2,3  coordinate index (x,y,z)
C
C     VOLDIR   = Volume of primitive cell
C
C     ATOM1(i) = Coordinates of first atom in the basis
C     ATOM2(i) = Coordinates of second atom in the basis
C                (The reference lattice site is at (0,0,0))
C-----------------------------------------------------------------------
```

and then the Reciprocal Lattice basis vectors

```
C-----------------------------------------------------------------------
C                                                      RECIPROCAL LATTICE
C-----------------------------------------------------------------------
C     CONSTR      = Lattice constant of reciprocal lattice
C     FACTOR      = Lattice constant / volume of primitive cell
C
C     RBASIS(i,j) = basis vectors of reciprocal lattice primitive cell
C                   (face centered cubic direct lattice)
C              i  = 1,2,3  vector index
C              j  = 1,2,3  coordinate index (x,y,z)
C
C     IMAX        = Maximum index for loops
C-----------------------------------------------------------------------
```

Then, a set of lattice vectors are constructed in reciprocal space, with coordinates in the arrays `GVECX`, `GVECY` and `GVECZ`. The solution matrix is dense. It is solved by using standard EISPACK routines `TRED1` and `TQLRAT`, included in the code. The bandstructure is calculated in a rectangular region of Brillouin zone, in correspondence of crystal momentum coordinates `BANDX`, `BANDY` and `BANDZ`, mapped by the indices `I1`, `I2`, `I3`. The number of crystal momentum points along each coordinate is fixed by NSTEP, with separation STEPK.

The code is written in plain FORTRAN for maximum portability. It should compile with little or no effort with any FORTRAN compiler.