1. Generate band structures, density of states, etc…

Calls cpw\_pp\_band\_dos.

* + - Use/reset dual approximation
    - Band structure
      * Preparation
        + Energy cutoff
      * Full PW diagonalization
      * Luttinger-Kohn basis (single k-point)
      * k.p method, including files for later plotting/use
      * GLK interpolation (2 k-point Luttinger-Kohn) with optional unfolding
      * Unfolding with PW diagonalization
      * Prepare file for later plotting, with unfolding and orbital information
    - Density of states
      * Full PW diagonalization
      * GLK interpolation (4 k-point Luttinger-Kohn)
      * k.p (not yet reimplemented)
    - Single k-vector
      * Number of bands
      * k-point
      * spin-orbit
        + eigenvalues
        + Eigenvalues and kinetic energy
        + Eigenvalues and eigenfunctions
        + Hamiltonian components
        + File for k.p
        + Oscillator strength
    - File for dielectric function
      * Normal diagonalization
        + Full PW, AO, AOJC diagonalization
        + Workers (should be elsewhere?)
      * GLK interpolation (4 k-point Luttinger-Kohn)

1. MTB

Calls ao\_interpolation\_sub.

* + - Use dual approximation
    - Use existing file (if it exists)
    - Preparation
      * interpolation mesh size
      * spin orbit
      * derivatives needed for dielectric function
    - Unfolded band structure
    - File for density of states
    - File for dielectric function
    - Wannier90 compatible file

1. Plot charge densities and potentials

Calls rho\_v\_plot\_sub.

* + - 1D (line plot) of plane averages, or double averages. Options are all the same only detailed for charge density.
      * Charge density
        + Interactive plots (in gnuplot, otherwise xmgr)
        + Number of lattice planes (for double average)
        + Choice of double average parameters
      * Bonding charge density
      * Effective potential
      * Hartree potential
      * XC potential
      * Ionic potential
    - 2D (contour plot)
      * FFT grid size
      * plot plane origin and edges
    - 3D using xsf format
      * FFT grid size

1. DOS from previous data

Calls dos\_sub.

* + - What range
      * Full range
      * Near the gap
      * Full control (will ask further questions)
    - Choose files
      * Defaults
      * Choose filename
    - Choose zero of energy
      * Average internal potential
      * Estimate of VBM
      * Estimate of CBM
      * Bottom of valence band
      * Fermi energy

1. Band structure from k.p data

Calls silvaco\_sub.

* + - (not yet updated)

1. Dielectric function from previous data

Calls ie\_sub.

* + - Which component (including all)
    - Spin-orbit